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Dislocation Microstructures and the Effective Behavior of Single Crystals

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Abstract

We consider single-crystal plasticity in the limiting case of infinite latent hardening, which signifies that the crystal must deform in single slip at all material points. This requirement introduces a nonconvex constraint, and thereby induces the formation of fine-scale structures. We restrict attention throughout to linearized kinematics and deformation theory of plasticity, which is appropriate for monotonic proportional loading and confers the boundary value problem of plasticity a well-defined variational structure analogous to elasticity.

We first study a scale-invariant (local) problem. We show that, by developing microstructures in the form of sequential laminates of finite depth, crystals can *beat* the single-slip constraint, i.e., the macroscopic (relaxed) constitutive behavior is indistinguishable from multislip ideal plasticity. In a second step, we include dislocation line energies, and hence a length scale, into the model. Different regimes lead to several possible types of microstructure patterns. We present constructions which achieve the various optimal scaling laws, and discuss the relation with experimentally known scalings, such as the Hall-Petch law.

1. Introduction

The effective behavior of ductile single crystals is the macroscopic manifestation of processes of crystallographic slip occurring on the scale of the crystal lattice, and is known to be mediated by the formation of dislocation structures. Such effective behavior includes yielding, work hardening rates and scaling laws such as the Hall-Petch relation [20, 44], i.e., the inverse square-root dependence of the yield stress on grain size in polycrystalline metals. In most crystals, slip occurs on well-characterized crystallographic planes and directions, known as *slip systems*. The observed microstructures often consist of ostensibly dislocation-free cells or lamellae in which a small number of slip systems is activated [46, 50, 37, 19, 48, 28, 26].

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This segregation of slip activity, or *patchy slip*, is closely connected with a fundamental property of ductile single crystals known as *latent hardening*, namely, that single crystals exhibit much higher rates of hardening in multiple slip than in single slip. Indeed, the phenomenon of latent hardening was inferred from the patchy slip patterns by PIERCY *et al.* who argued that "*these results prove the reality of latent-hardening, in the sense that the slip lines of the one system experience difficulty in breaking through the active slip lines of the other one*" [46, p. 337]. This conjectured connection between strong latent hardening and patchy slip was born out by the finite-element calculations of PIERCE *et al.* [45], where single-crystal specimens endowed with strong latent hardening and subjected to uniaxial tension exhibit non-uniform slip patterns consisting of alternating regions of single slip.

The strong latent-hardening property of ductile single crystals has been quantified by means of specially designed experiments [31, 16, 17, 54, 5]. The presence of strong latent hardening implies that crystals have an incentive, in work of deformation terms, to deform in single slip and avoid multiple slip. More precisely, the work of deformation expended in deforming a crystal into a deformation field composed of regions of single slip may be less than the work or deformation required to attain the same average or macroscopic deformation by multiple slip [42, 43]. ORTIZ & REPETTO [42] showed that strong latent hardening renders the incremental variational problem of single-crystal plasticity nonconvex, and on this basis they argued that microstructural formation in ductile single crystals is a manifestation of non-attainment.

An additional fundamental property of single crystals is the dependence of their behavior on the size of the sample, be it the grain size, wire diameter, film thickness, or some other limiting feature size. This dependence is sometimes referred to as *size effect*. A classical manifestation of this size effect is the aforementioned Hall-Petch effect. Material models which are sensitive to the size of the sample are necessarily nonlocal and contain intrinsic length-scale parameters. The intrinsic length scale which renders the behavior of crystals nonlocal is the length scale of the atomic lattice. Indeed, the core energy of the dislocations depends sensitively on the Burgers vector, whose length is in turn commensurate with the lattice parameter. ORTIZ *et al.* [42, 43, 4] have shown that consideration of core energies results in scaling behavior consistent with the Hall-Petch relation and with experimental observations of the dependence of the microstructural size on macroscopic deformation [55, 6, 27, 26, 25, 21].

In this paper we address two main problems concerning:

(P1) The effective constitutive behavior of single crystals in the local approximation.
(P2) The dependence of the behavior of crystals on the sample geometry.

The chief analysis tool which we bring to bear on problem (P1) is relaxation, whereas the main objective in connection with problem (P2) is the determination of optimal scaling laws. In related, but different, problems this kind of scaling result has been studied in the physics literature [34, 35, 24, 47] and more recently mathematically in [32, 33, 10, 11, 13, 29, 7, 12]. In order to facilitate the analysis we make a number of simplifying assumptions. Firstly, we restrict attention

throughout to linearized kinematics and deformation theory of plasticity. This latter theory of plasticity is obtained when all material points are assumed to follow certain optimal deformation paths (see, e.g., [36] and references therein) and confers to the boundary value problem of plasticity a well-defined variational structure analogous to elasticity. Deformation theory of plasticity provides an appropriate description of plastic solids deforming under the action of monotonic proportional loading. Secondly, we shall assume that the crystals exhibit no hardening, or ideal plasticity, in single slip. This assumption is justified as most crystals exhibit easy glide, i.e., low or vanishing rates of hardening, in single slip. Finally, following [42, 4] for simplicity we study the limiting case of crystals exhibiting infinitely strong latent hardening. We take this property to signify that the crystal must necessarily deform in single slip at all material points. This requirement introduces a nonconvex constraint which renders the variational problem nonconvex.

The main results of the paper are as follows. We show that, by developing microstructures in the form of sequential laminates of finite depth, crystals can *beat* the single-slip constraint, i.e., their relaxed constitutive behavior is indistinguishable from multislip ideal plasticity. We find, however, that for some average deformations relaxation of the single-slip constraint requires the formation of concentrated slip in the microstructure, such as occurs in *slip lines*, i.e., lines of concentrated slip and discontinuous displacement. Including dislocation line energies in the model, we find that the results become scale-dependent, and different patterns are formed in different regimes. We present constructions which lead to various optimal scaling laws, and discuss the relation with experimentally known scalings.

2. The variational problems of single-crystal plasticity

In this section we define the variational problems which govern deformations of a ductile single crystal occupying a domain $\Omega \subset \mathbb{R}^3$. We shall assume throughout linearized kinematics and we let $u : \Omega \to \mathbb{R}^3$ be the displacement field, $\beta(u) = \nabla u : \Omega \to \mathbb{R}^{3\times 3}$ the displacement-gradient field, and $\epsilon(u) : \Omega \to \mathbb{R}^{3\times 3}_{\rm sym}$ the strain field corresponding to u, which is defined by

$$\epsilon(u) = \beta^{\rm sym} = \nabla u^{\rm sym}.$$

Here and below, $\beta^{\rm sym} = (\beta + \beta^T)/2$ denotes the symmetric part of a matrix β. Plastic deformation in single crystals is crystallographic in nature, and, for monotonic deformations, the plastic distortion tensor admits the representation

$$\beta^p(\gamma) = \sum_{i=1}^{N} \gamma_i \, s_i \otimes m_i,$$

where $\gamma_i \in \mathbb{R}$ is the slip strain on system i, s_i and m_i are the slip direction and plane normal corresponding to slip system i, respectively, N is the number of slip systems and $\otimes$ denotes the dyadic product of two vectors, $(a \otimes b)_{ij} = a_i b_j$. We

System	B2	B4	B5	A3	A2	A6
Direction	$\pm[0\bar{1}1]$	$\pm[10\bar{1}]$	$\pm[\bar{1}10]$	$\pm[101]$	$\pm[01\bar{1}]$	$\pm[\bar{1}\bar{1}0]$
Plane	(111)	(111)	(111)	$(\bar{1}11)$	$(\bar{1}11)$	$(1\bar{1}1)$
System	C1	C3	C5	D4	D1	D6
Direction	$\pm[011]$	$\pm[\bar{1}0\bar{1}]$	$\pm[1\bar{1}0]$	$\pm[\bar{1}01]$	$\pm[0\bar{1}\bar{1}]$	$\pm[110]$
Plane	$(\bar{1}\bar{1}1)$	$(\bar{1}1\bar{1})$	$(\bar{1}\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$

Table 2.1. The set $\mathcal{S}$ of slip systems for fcc crystals relative to the cubic axes, and Schmid and Boas' nomenclature. For each slip system, the slip direction s and the slip-plane normal m are given.

System	Direction	Plane	System	Direction	Plane
$A2$	$[\bar{1}11]$	$(0\bar{1}1)$	$A2'$	$[\bar{1}11]$	(211)
$A3$	$[\bar{1}11]$	(101)	$A3'$	$[\bar{1}11]$	$(12\bar{1})$
$A6$	$[\bar{1}11]$	(110)	$A6'$	$[\bar{1}11]$	$(1\bar{1}2)$
$B2$	[111]	$(0\bar{1}1)$	$B2''$	[111]	$(\bar{2}11)$
$B4$	[111]	$(\bar{1}01)$	$B4'$	[111]	$(1\bar{2}1)$
$B5$	[111]	$(\bar{1}10)$	$B5'$	[111]	$(11\bar{2})$
$C1$	$[11\bar{1}]$	$(0\bar{1}1)$	$C1'$	$[11\bar{1}]$	$(2\bar{1}1)$
$C3$	$[11\bar{1}]$	(101)	$C3''$	$[11\bar{1}]$	$(\bar{1}21)$
$C5$	$[11\bar{1}]$	$(\bar{1}10)$	$C5''$	$[11\bar{1}]$	(112)
$D1$	$[1\bar{1}1]$	$(0\bar{1}1)$	$D1''$	$[1\bar{1}1]$	$(21\bar{1})$
$D4$	$[1\bar{1}1]$	$(\bar{1}01)$	$D4''$	$[1\bar{1}1]$	(121)
$D6$	$[1\bar{1}1]$	(110)	$D6''$	$[1\bar{1}1]$	$(\bar{1}12)$

Table 2.2. The set $\mathcal{S}$ of slip systems for bcc crystals relative to the cubic axes, and Schmid and Boas' nomenclature. For each slip system, the slip direction s and the slip-plane normal m are given.

shall denote the set of slip systems $\{s_i \otimes m_i\}_{i=1..N}$ by $\mathcal{S}$. The corresponding plastic strain is

$$\epsilon^p(\gamma) = (\beta^p(\gamma))^{\text{sym}} = \frac{1}{2}\Big[\beta^p(\gamma) + \beta^{pT}(\gamma)\Big].$$

Plastic deformations resulting from conservative glide of dislocations are characterized by slip directions contained within the slip plane, and correspondingly do not change the specific volume of the material, i.e.,

$$s_i \cdot m_i = 0.$$

The slip systems of the various crystal classes have been determined experimentally (e.g., [23]). Face-centered cubic (fcc) crystals typically show activity on the twelve slip systems belonging to the class of {111} planes and [110] directions, listed in Table 2.1, whereas body-centered cubic (bcc) crystals show activity in the twenty-four systems consisting of planes in the classes {211} and {110} and slip directions of type [111], listed in Table 2.2.

In order to further streamline the analysis we shall idealize crystals as possessing no self-hardening and infinite latent hardening. These assumptions lead to the consideration of a stored plastic-work function of the form

$$W^p(\gamma) = \begin{cases} \tau_i|\gamma_i| \text{ if } \gamma_j = 0, & \forall j \neq i, \\ \infty \quad \text{else}, \end{cases}$$

where τ_i is the critical resolved shear stress of the crystal. All symmetry-related systems have the same value of τ_i, so that for example in fcc crystals there is only one value of τ. We note that, owing to the infinite latent-hardening assumption, W^p is infinity for plastic deformations other than single-slip deformations of the form

$$\beta^p(\gamma) = \gamma_i s_i \otimes m_i$$

for some $i \in \{1, \ldots, N\}$ and slip strain $\gamma_i \in \mathbb{R}$. The free-energy density of the crystal is

$$A(\beta, \gamma) = \tfrac{1}{2}\,(C\,(\epsilon - \epsilon^p(\gamma)), (\epsilon - \epsilon^p(\gamma))) + W^p(\gamma),$$

where C is the matrix of the elastic moduli of the crystal, which is assumed constant and positive definite, and as above $\epsilon = \beta^{\mathrm{sym}}$. Finally, the strain-energy density of a uniformly deformed crystal at displacement gradient $\nabla u = \beta =$ constant is

$$W(\beta) = \min_{\gamma \in \mathbb{R}^N} A(\beta, \gamma)\,. \tag{2.1}$$

We note that $W(\beta)$ vanishes for linearized rotations, i.e, $W(\omega) = 0$ for all $\omega \in so(3) = \{\omega \in \mathbb{R}^{3\times 3} : \omega = -\omega^T\}$. Further, $W(\beta)$ has linear growth along the single-slip orbits

$$\beta = \gamma_i s_i \otimes m_i + \omega$$

(for some $i \in \{1, \ldots, N\}$ and $\omega \in so(3)$), and quadratic growth in all other directions.

In Section 3 we study the relaxation of the local energy functional

$$I(u) = \int_\Omega W(\nabla u) dx\,. \tag{2.2}$$

By local we mean that the energy density only depends on the strain ∇u and does not contain, for example, strain-gradient terms. This makes the problems scale-invariant. It is worth mentioning that standard theory shows that the relaxation $J(u)$ of $I(u)$ extends in the obvious way in the presence of continuous perturbations such as body forces (e.g., [15, 8], we use here the strong L^1 topology, see Section 3). The results obtained below are thus applicable to the general boundary value problem which governs the quasistatic deformations of single crystals subjected to body forces and displacement boundary conditions on part of $\partial\Omega$. Standard theory also provides a compelling connection between the minimizers of $J(u)$ and $I(u)$. Thus, for instance, if $I(u)$ is coercive, it follows that $J(u)$ is also coercive and lower semicontinuous and, hence, has a minimum point in an appropriate larger space X. Furthermore, $\inf_{u\in X} I(u) = \inf_{u\in X} J(u)$ and every cluster point of a minimizing sequence of $I(u)$ is a minimum point of $J(u)$ in X. Finally, every minimum point of $J(u)$ is the limit of a minimizing sequence of $I(u)$ in X. These properties of relaxation show that, if one is interested in the macroscopic behavior, the functional

$I(u)$ can be replaced without loss of information by the better-behaved functional $J(u)$. Indeed, minimizing sequences of $I(u)$ correspond to *microstructures*, and minimizers of $J(u)$ characterize their average properties.

The local functional (2.2) lacks an intrinsic length scale and, consequently, cannot predict microstructural sizes. In particular, the relaxed functional $J(u)$ is itself local and independent of the choice of domain Ω. The local character of the theory is lost as soon as the core energy of the dislocations is taken into account, since consideration of core energies brings an intrinsic length into the theory, namely, the lattice parameter. The connection between deformation fields and dislocation structures may be established readily by recourse to the theory of continuously distributed dislocations (e.g., [39]). While the displacement-gradient field $\beta(x)$ is subject to compatibility requirements, the plastic-distortion field $\beta^p(x)$ need not be compatible in general. Following NYE [40], the dislocation density tensor is defined as

$$\alpha = \operatorname{curl} \beta^p(\gamma) \tag{2.3}$$

or, in components, $\alpha_{lk} = \beta^p_{li,j}\varepsilon_{jik}$, with ε_{jik} denoting the components of the permutation tensor. It is evident from (2.3) that α is a measure of the incompatibility of β^p. Following [42, 43], the dislocation core energy may be taken into account by means of a simple line-tension model. This extension results in the functional

$$E(u,\gamma) = \int_\Omega \left[A(\nabla u, \gamma) + \frac{T}{b} \left| \operatorname{curl} \beta^p(\gamma) \right| \right] dx, \tag{2.4}$$

where T is the dislocation line tension and b is the Burgers vector length, which is of the order of the lattice parameter. It is readily verified that, when α represents a collection of discrete dislocation lines, the second term in the energy (2.4) is T times the total dislocation length in Ω, as required. The nonlocal functional (2.4) is discussed in Section 4, under some additional simplifying assumptions on the active set of slip systems.

3. Relaxation of the local energy

Let $\Omega \subset \mathbb{R}^3$ be a bounded Lischitz domain, and $\Gamma \subset \partial\Omega$ an open subset of its boundary on which we impose Dirichlet boundary conditions. For a given u_0, we consider the functional

$$I_\Gamma(u) = \begin{cases} \int_\Omega W(\nabla u) dx & \text{if } u \in W^{1,2}(\Omega, \mathbb{R}^3), \quad u = u_0 \text{ on } \Gamma, \\ \infty & \text{else,} \end{cases} \tag{3.1}$$

where the energy density W was defined in (2.1). Here and in the following, the values on Γ are understood in the sense of traces, and u_0 is assumed to have enough regularity for the functional to make sense. This means $u_0 \in H^{1/2}(\Gamma)$ for $I(u)$, the relaxed functional will allow for u_0 in the larger space $L^1(\Gamma)$. An additional term containing body tractions of the form

$$T(u) = \int_\Omega u \cdot f \; dx$$

for some fixed $f \in L^\infty(\Omega)$ is a continuous perturbation of I, and can be included without any change in all statements, since the topology used here is stronger than L^1 (see below). Precisely, if $J(u)$ is the relaxation of $I(u)$, then $J(u) + T(u)$ will be the relaxation of $I(u) + T(u)$. A similar continuity result holds, in general, for the case of surface tractions, and such a term is well defined since all finite-energy u have a trace in $L^1(\partial\Omega)$. However, since the functional has linear growth, strong surface tractions can disrupt coercivity, and even positivity, of the functional. Hence only weak surface tractions can be seen as a continuous perturbation, see e.g. [3] (this corresponds to the so-called safe-load condition).

The functional $I(u)$ is not lower semicontinuous, and minimizing sequences form fine-scale oscillations. Indeed, the energy density W only allows for single-slip plastic deformation, whereas a variety of multiple-slip deformations can be obtained by mixing on a fine scale different single-slip deformations. The aim of this section is to obtain the relaxation of (3.1), which describes the macroscopic material behavior, averaged over such fine-scale structures. We recall that it is characterized by the two properties:

(i) Lower bound. For each sequence u_h converging to u, we have

$$J(u) \leqq \liminf_{h\to\infty} I(u_h)\,.$$

(ii) Recovery sequence. For each u, there is a sequence u_h converging to u such that

$$J(u) = \lim_{h\to\infty} I(u_h)\,.$$

We now specify the topology for the mentioned convergences and the space on which J is defined. Both are determined by the coerciveness of the original functional $I(u)$. In particular, since

$$W(\beta) \geqq c|\beta^{\mathrm{sym}}| + c|\operatorname{Tr}\beta|^2\,, \tag{3.2}$$

we know that, on any low-energy sequence u_h, $\operatorname{div} u_h$ is uniformly bounded in L^2, and $\nabla u_h^{\mathrm{sym}}$ in L^1. However, $W(\nabla u)$ is independent of the antisymmetric part of ∇u, and control of $\nabla u_h^{\mathrm{sym}}$ in L^1 does not imply an analogous control of ∇u_h in L^1 (recall that Korn's inequality does not hold in L^1, see [41, 14]). The appropriate space, whose norm corresponds directly to the one entering (3.2), is

$$U(\Omega) = \left\{ u \in BD(\Omega, \mathbb{R}^3) : \operatorname{div} u \in L^2(\Omega) \right\}$$

(see [51, 53]). We recall that the space BD is defined as the set of L^1 functions whose symmetrized distributional gradient $Eu = Du + Du^T$ is a finite measure. The spaces $BD(\Omega)$ and $U(\Omega)$ have been introduced and studied in the context of Hencky plasticity [51, 2, 53, 3, 22, 52, 9, 1], where the energy density has the same coercivity properties stated in (3.2), but is convex. The theory of the functions of bounded deformation proceeds in many ways analogously to the one of functions of bounded variation (i.e., those for which the full gradient Du is a finite measure), but BD is a strictly larger space, and several fine properties are still open [1].

All low-energy sequences for $I(u)$ are uniformly bounded in $U(\Omega)$, with the seminorm

$$\|u\|_{U(\Omega)} = \|\operatorname{div} u\|_{L^2(\Omega)} + |Eu|(\Omega)\,,$$

and by a standard compactness result [53, 2] they have a subsequence that converges strongly in L^1 (up to global translations). Therefore in the definition of the relaxation we can use the topology given by the L^1 norm. The two properties characterizing $J(u)$ show then that J is lower semicontinuous with respect to the strong L^1 convergence. By the above argument, the very same topology makes minimizing sequences of I (and hence of J) compact, hence we immediately obtain existence of minimizers for J.

The determination of the relaxation of $I(u)$ is based on the determination of the appropriate envelope for the energy density W. Since W does not have a uniform growth at infinity, standard results do not apply. We present here an explicit derivation of the relaxation, where this difficulty is circumvented by resorting to convexity. We start by a definition of the quasiconvex envelope W^{qc},

$$W^{\mathrm{qc}}(\beta) = \inf\left\{\int_{(0,1)^3} W(\nabla u)\,dx : u \in W^{1,\infty},\ u(x) = \beta x \text{ on } \partial(0,1)^3\right\} \quad (3.3)$$

(see, e.g., [38]). This definition shows that replacing W by W^{qc} amounts to optimizing over all possible gradient fields with given boundary values. The concept of quasiconvexity was introduced by Morrey in 1952 to study existence for variational problems depending on a gradient field, and has proved very useful in the analysis of solid-solid phase transitions (see, e.g., [38, 30] and references therein). In general, the quasiconvex envelope is different from the convex one, and much more difficult to compute. Indeed, only for very few realistic energies W has the analytic expression for W^{qc} been found. In the present case, we shall show that (under some assumptions on the set of slip systems) the quasiconvex envelope coincides with the convex envelope W^{**}. This will be the key ingredient for the explicit evaluation of the relaxation $J(u)$.

We start from a characterization of W^{**}, which corresponds to averaging over all possible local strain distributions, neglecting the gradient constraint. The same energy W^{**} is obtained if latent hardening is neglected (Section 3.1). Then we discuss some simple mixtures which satisfy the gradient constraint, called laminates, and present our kinematic assumption on the set of slip systems $\mathcal{S}$ (Section 3.2). In Section 3.3 we turn to the full problem $I(u)$, and give its relaxation first without boundary conditions (i.e., assuming that $\Gamma = \emptyset$), which is simpler to obtain. The equality of the quasiconvex and convex envelopes is proved in Section 3.4, and the applicability of our result to fcc and bcc crystals in Section 3.5. Finally, in Section 3.6 we discuss the minimal complexity of the microstructure patterns for some specific average shears, and, in Section 3.7, we generalize the relaxation of $J(u)$ to the case where Dirichlet boundary conditions are imposed.

3.1. The convex envelope

The convex envelope of W is defined as usual by

$$W^{**}(\beta) = \inf\left\{\sum_i \lambda_i W(\beta_i) : \lambda_i \geqq 0,\ \sum_i \lambda_i = 1,\ \beta_i \in \mathbb{R}^{3\times 3}\right\}.$$

Replacing W with W^{**} in the energy density $I(u)$ corresponds to neglecting latent hardening, i.e., to permitting each material point to deform at the same time along several slip systems (multislip plasticity). In particular, W^{**} corresponds to optimizing locally over all mixtures between the different slip systems, without considering the gradient constraint.

Lemma 3.1. *With the above definitions, a positive-definite elasticity matrix C, and a set of slip systems $\mathcal{S}$ such that $(s_i \otimes m_i)^{\mathrm{sym}}$ span the set of traceless symmetric matrices, the following holds:*

(i) The envelope W^{**} satisfies

$$W^{**}(\beta) = \min_{\gamma\in\mathbb{R}^N} A^{**}(\beta, \gamma) \tag{3.4}$$

where A^{**} is the convex envelope of A, and satisfies

$$A^{**}(\beta, \gamma) = \frac{1}{2}\left(C\left(\epsilon - \epsilon^p(\gamma)\right), \left(\epsilon - \epsilon^p(\gamma)\right)\right) + \sum_i \tau_i |\gamma_i|. \tag{3.5}$$

Here $\epsilon = \beta^{\mathrm{sym}}$ and $\epsilon^p(\gamma) = \sum \gamma_i (s_i \otimes m_i)^{\mathrm{sym}}$.

(ii) The envelope W^{**} has linear growth on traceless symmetric matrices and quadratic on the trace; precisely, there are constants c, c' such that

$$c\left(|\beta^{\mathrm{sym}}| + |\operatorname{Tr}\beta|^2 - 1\right) \leqq W^{**}(\beta) \leqq c'\left(1 + |\beta^{\mathrm{sym}}| + |\operatorname{Tr}\beta|^2\right). \tag{3.6}$$

Proof. Equation (3.4) is a direct consequence of the following general fact. For $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$, let $f(x) = \inf_y g(x, y)$. Then, the convex envelopes satisfy $f^{**}(x) = \inf_y g^{**}(x, y)$. To see this, observe that by definition

$$\begin{aligned} f^{**}(x) &= \inf\left\{\sum_i \lambda_i f(x_i) : \sum_i \lambda_i x_i = x\right\} \\ &= \inf\left\{\sum_i \lambda_i g(x_i, y_i) : \sum_i \lambda_i x_i = x,\ \ y_i \in \mathbb{R}^m\right\}, \end{aligned}$$

where the λ_i's are implicitly assumed to be nonnegative weights with sum one. On the other hand,

$$g^{**}(x, y) = \inf\left\{\sum_i \lambda_i g(x_i, y_i) : \sum_i \lambda_i x_i = x,\ \ \sum_i \lambda_i y_i = y\right\}.$$

By taking $f = W$, $g = A$, we obtain (3.4). Attainment follows from continuity of A^{**} and the growth $A^{**}(\beta, \gamma) \geqq c|\gamma|$.

We now show that the convex envelope of A is given by (3.5). Indeed, let $\tilde{A}$ be the function defined in the right-hand side of (3.5). Since $\tilde{A}$ is convex and less than or equal to A, we get $\tilde{A} \leqq A^{**}$. To show equality, fix some (β, γ), and consider the convex combination given by

$$\lambda_i = \frac{|\gamma_i|}{\sum_j |\gamma_j|}, \qquad \gamma^{(i)} = \sum_j |\gamma_j| \frac{\gamma_i}{|\gamma_i|} e_i, \qquad \beta^{(i)} = \beta - \epsilon^p(\gamma) + \epsilon^p(\gamma^{(i)}).$$

A straightforward computation shows that

$$\sum \lambda_i = 1, \qquad \sum \lambda_i \gamma^{(i)} = \gamma, \qquad \sum \lambda_i \beta^{(i)} = \beta,$$
$$\sum \lambda_i A(\beta^{(i)}, \gamma^{(i)}) = \tilde{A}(\beta, \gamma),$$

hence $\tilde{A} \geqq A^{**}$ and (3.5) is proved.

The growth condition (3.6) follows from the fact that the slip systems $(s_i \otimes m_i)^{\text{sym}}$ span the set of symmetric traceless matrices, and that $c|\epsilon|^2 \leqq (C\epsilon, \epsilon) \leqq c'|\epsilon|^2$. This concludes the proof. □

3.2. Laminates and completeness of the set of slip systems $\mathcal{S}$

Even if ∇u is locally a single-slip deformation, the formation of fine-scale structures permits us to obtain macroscopic (average) plastic deformations which are not single-slip. However, those structures must obey the gradient constraint, i.e., only those mixtures which are curl-free can be realized by $\beta = \nabla u$. The prototype is a laminate, which is a mixture between two gradients, whose difference is a rank-one matrix. Given two strains β_1 and β_2, with $\beta_2 - \beta_1 = a \otimes n$, two nonnegative weights λ_1, λ_2, with $\lambda_1 + \lambda_2 = 1$, and a small $\varepsilon > 0$, we write

$$u_\varepsilon(x) = \beta_1 x + a\varepsilon \chi\left(\frac{x \cdot n}{\varepsilon}\right),$$

where $\chi : \mathbb{R} \to \mathbb{R}$ is defined by $\chi(0) = 0$, $\chi'(t) = 0$ if $t \in (k, k + \lambda_1)$ and $\chi'(t) = 1$ if $t \in (k + \lambda_1, k + 1)$, for $k \in \mathbb{Z}$. For small ε, ∇u oscillates on a fine scale between the values β_1 and β_2, with average $\beta = \lambda_1\beta_1 + \lambda_2\beta_2$. As $\varepsilon \to 0$, the sequence $u_\varepsilon(x)$ converges weakly-$*$ in $W^{1,\infty}$ to an affine function with gradient β. This shows that mixtures are always possible between rank-one connected matrices. This construction is called a first-order laminate; iterating the procedure we can construct laminates of higher order (see below).

Due to the linearized rotational invariance, only the symmetric part of the gradient is relevant for the energy. In particular, we can replace β_2 with $\beta_2' = \beta_2 + \omega$, for any $\omega \in so(3)$, and generalize the condition above to the existence of ω, a and n such that $\beta_2 - \beta_1 = a \otimes n + \omega$. The latter condition depends only on the symmetric part of β_1 and β_2, which we denote by $\epsilon_i = \beta_i^{\text{sym}}$. We say that two symmetric matrices ϵ_1 and ϵ_2 are *symmetrically rank-one connected* if there are vectors a and

n such that $\epsilon_1 - \epsilon_2 = a \otimes n + n \otimes a$. A straightforward calculation shows that ϵ_1 and ϵ_2 are symmetrically rank-one connected if and only if $\det(\epsilon_1 - \epsilon_2) = 0$.

Iteration of this construction leads to the determination of the lamination convex hull of a set. More precisely, given a set K of symmetric matrices, we define $K^{\mathrm{slc},0} = K$ and iteratively $K^{\mathrm{slc},i+1}$ as the set of symmetrized averages of laminates between matrices in $K^{\mathrm{slc},i}$, precisely,

$$K^{\mathrm{slc},i+1} = \left\{ \epsilon : \quad \epsilon \in [\epsilon_1, \epsilon_2],\ \epsilon_1,\ \epsilon_2 \in K^{\mathrm{slc},i}, \quad \det(\epsilon_1 - \epsilon_2) = 0 \right\},$$

where $[\epsilon_1, \epsilon_2]$ denotes the segment whose endpoints are ϵ_1 and ϵ_2. The union of all $K^{\mathrm{slc},i}$ constitutes the symmetric lamination convex hull of K, which we call K^{slc} (with this definition, only finitely many iterations are permitted). All strains in K^{slc} can be obtained as average gradients of maps whose strains lie in K (up to negligible boundary terms).

We now state our main assumption on the set of slip systems $\mathcal{S}$, which is of purely kinematic nature.

Definition 3.2. A set of slip systems $\mathcal{S} = \{s_i \otimes m_i\}$ is *complete* if the symmetric lamination convex hull of the finite set

$$\left\{ \pm (s_i \otimes m_i)^{\mathrm{sym}} : \ s_i \otimes m_i \in \mathcal{S} \right\}$$

contains a neighborhood of the origin in the space of symmetric traceless matrices.

This corresponds to the attainability of all (infinitesimally) volume-preserving deformations by suitable combinations of the slip systems. This condition can be replaced by a more general but less explicit one replacing the lamination hull with the quasiconvex one, leading to essentially the same conclusions, at the expense of a more technical discussion. For simplicity we focus here on the simpler condition involving lamination convexity. We show in Section 3.5 that the slip systems of fcc and bcc metals do satisfy this definition, and that complenetess is not equivalent to $(s_i \otimes m_i)^{\mathrm{sym}}$ spanning the set of traceless symmetric matrices.

3.3. The relaxation of $I(u)$ without boundary conditions

We now present the relaxation result without boundary conditions. The generalization to the case of Dirichlet boundary conditions will be presented in Section 3.7 below. The relaxed functional is finite on functions $u \in U(\Omega)$, whose symmetrized distributional gradient $Eu = Du + Du^T$ can be decomposed as usual by $Eu = \mathcal{E}u dx + E_s u$, where $\mathcal{E}u$ is the density of the continuous part of Eu with respect to the Lebesgue measure, and $E_s u$ the part of Eu orthogonal to it (called the singular part). Since functions in $U(\Omega)$ have a divergence in L^2, it follows that the singular part E_s is traceless. The continuous part $\mathcal{E}$ enters then the relaxed functional through the convex envelope W^{**} of W, and the singular part E_s through its regression function, defined by

$$W^{\infty}(\beta) = \lim_{t \to \infty} \frac{1}{t} W^{**}(t\beta).$$

The limit exists since W^{**} is convex, and is finite for all traceless β by the growth condition (3.6).

Theorem 3.3. *Let W be as in* (2.1)*, with a positive definite elasticity matrix C, and the set of slip systems $\mathcal{S}$ be complete. Then, the relaxation of*

$$I(u) = \begin{cases} \displaystyle\int_\Omega W(\nabla u)dx & \text{if } u \in W^{1,2}(\Omega, \mathbb{R}^3) \\ \infty & \text{else} \end{cases}$$

with respect to the strong L^1 topology is given by

$$J(u) = \begin{cases} \displaystyle\int_\Omega W^{**}(\mathcal{E}u)dx + \int_\Omega W^\infty\left(\frac{E_s u}{|E_s u|}\right) d|E_s u| & \text{if } u \in U(\Omega), \\ \infty & \text{else.} \end{cases}$$

The proof is based on matching upper and lower bounds. The lower bound is obtained by proving that $J(u)$ is a convex functional of the measure Eu, and that it is less than or equal to $I(u)$. Convexity of functionals depending on convex functions with linear growth is a classical result. Precisely, if $f : \mathbb{R}^m \to \mathbb{R}$ is a convex function and $0 \leqq f(\xi) \leqq c(1 + |\xi|)$, and μ_h is a sequence of $\mathbb{R}^m$-valued Radon measures on Ω converging weakly in $\mathcal{M}$ to μ, such that $\int_\Omega d|\mu_h|$ is bounded, then

$$\begin{aligned} \liminf_{h\to\infty} \int_\Omega f\left(\frac{d\mu_h}{dx}\right) dx + \int_\Omega f^\infty\left(\frac{d\mu_h^s}{d|\mu_h^s|}\right) d|\mu_h^s| \\ \geqq \int_\Omega f\left(\frac{d\mu}{dx}\right) dx + \int_\Omega f^\infty\left(\frac{d\mu^s}{d|\mu^s|}\right) d|\mu^s|\,. \end{aligned} \tag{3.7}$$

Further, if $\int_\Omega |\mu| = \lim \int_\Omega |\mu_h|$, then equality holds (see, e.g., Theorem 1.3 in [9]; the result was first proved in [18, 49]). In applying this result to our problem, care needs only to be taken to separate the volumetric part (which gives quadratic growth for the energy) from the deviatoric part (which gives linear growth). Here and below we say that a sequence of measures μ_h converges to μ weakly in $\mathcal{M}$ if

$$\int_\Omega \psi \; d\mu_h \to \int_\Omega \psi \; d\mu \text{ for every } \psi \in C_0^0(\Omega)\,.$$

To obtain the upper bound, we need to construct recovery sequences u_h. Due to a density argument, it is sufficient to do it for smooth limits u, which in particular have bounded gradients. We can therefore use the standard tools of quasiconvexity, which are typically applied for the relaxation of functionals depending on a gradient field, but which require higher regularity than BD (typically, $W^{1,p}$ with $p > 1$). The quasiconvex envelope is actually identical to the convex one, as will be shown in Proposition 3.4 below.

Proof. We start from the lower bound. Let u_h be a sequence of functions in $W^{1,2}(\Omega)$ converging to $u \in U(\Omega)$. Without loss of generality we can assume that $\lim I(u_h)$ exists and is finite. Since $W^{**} \leqq W$, we can use the coercivity part of (3.6), and by compactness choose a subsequence such that

$$u_h \to u \text{ strongly in } L^1\,, \qquad \operatorname{div} u_h \rightharpoonup \operatorname{div} u \text{ weakly in } L^2\,,$$

$$Eu_h \rightharpoonup Eu \text{ weakly in } \mathcal{M}.$$

We now decompose all strains in deviatoric and volumetric parts, according to the metric induced by the elasticity matrix C. To do this, let p denote a symmetric matrix such that

$$\operatorname{Tr} p = 1 \quad \text{and} \quad (Cp, \epsilon) = 0 \quad \text{for all } \epsilon \text{ such that } \operatorname{Tr}\epsilon = 0.$$

Any symmetric matrix ϵ can be written as

$$\epsilon = \epsilon^D + \epsilon^V p \qquad \text{where} \qquad \operatorname{Tr}\epsilon^D = 0 \text{ and } \epsilon^V = \operatorname{Tr}\epsilon \in \mathbb{R}\,. \tag{3.8}$$

The C-orthogonality guarantees that the energy is additive, in the sense that

$$W^{**}(\epsilon^D + \epsilon^V p) = W^{**}(\epsilon^D) + W^{**}(\epsilon^V p)\,. \tag{3.9}$$

To see this, observe that for any γ we have $A^{**}(\epsilon^D + \epsilon^V p, \gamma) = A^{**}(\epsilon^D, \gamma) + A^{**}(\epsilon^V p, 0)$. Taking the minimum over γ we get $W^{**}(\epsilon^D + \epsilon^V p) = W^{**}(\epsilon^D) + A^{**}(\epsilon^V p, 0)$. The last term equals $W^{**}(\epsilon^V p)$, since

$$A^{**}(\epsilon^V p, \gamma') = A^{**}(\epsilon^V p, 0) + \sum \tau_i |\gamma_i'| + \frac{1}{2}(C\epsilon^p(\gamma'), \epsilon^p(\gamma')) \geqq A^{**}(\epsilon^V p, 0)\,.$$

This concludes the proof of (3.9).

We now perform an analogous decomposition on the strains Eu_h and Eu, and denote as above by $\mathcal{E}$ the corresponding densities with respect to the Lebesgue measure, so that for example $Eu_h = E^D u_h + E^V u_h = \mathcal{E}^D u_h dx + \mathcal{E}^V u_h dx$. Since the decomposition is linear, the strains Eu_h have no singular part, and the volumetric parts are controlled in L^2, we get

$$\mathcal{E}^D u_h dx \rightharpoonup E^D u \text{ weakly in } \mathcal{M}\,, \quad \text{and} \quad \mathcal{E}^V u_h \rightharpoonup \mathcal{E}^V u \text{ weakly in } L^2\,.$$

The energy $W^{**} \leqq W$ has linear growth in the deviatoric part $\mathcal{E}^D u_h$, hence the lower semicontinuity result of (3.7) gives

$$\int_\Omega W^{**}(\mathcal{E}^D u)dx + \int_\Omega W^\infty\left(\frac{E_s u}{|E_s u|}\right) d|E_s u| \leqq \liminf_{h\to\infty} \int_\Omega W(\mathcal{E}^D u_h)dx\,.$$

On the other hand, on volumetric strains $W^{**}(\epsilon^V p) = |\epsilon^V|^2 W^{**}(p)$ is equivalent to the L^2 norm, hence is lower semicontinuous under weak-L^2 convergence. Recalling the additivity (3.9), we get

$$J(u) \leqq \liminf_{h\to\infty} \int_\Omega W^{**}(\mathcal{E}u_h)\,dx \leqq \liminf_{h\to\infty} I(u_h)\,.$$

This concludes the proof of the lower bound.

We now come to the upper bound. We remark that the construction presented here does not change the boundary values, and can therefore be reused later in the proof of Theorem 3.13 below.

First, by a general density argument, we reduce to smooth functions. Indeed, for any $u \in U(\Omega)$, there is a sequence $u_h \in C^\infty(\Omega) \cap U(\Omega)$ such that the following holds:

$$u_h \to u \text{ strongly in } L^1\,, \qquad \operatorname{div} u_h \to \operatorname{div} u \text{ strongly in } L^2\,,$$

$$Eu_h \rightharpoonup Eu \text{ weakly in } \mathcal{M}\,, \quad \int_\Omega |Eu_h| \to \int_\Omega |Eu|\,, \quad u_h = u \text{ on } \partial\Omega \text{ as traces}$$

(see, e.g., Theorem A.2 in [22] or Theorem II.3.4 in [52]).

As in the lower bound, we decompose all strains into volumetric and deviatoric parts, according to (3.8). The strong convergence of $\operatorname{div} u_h$ gives $\int W^{**}(p \operatorname{div} u_h)dx \to \int W^{**}(p \operatorname{div} u)dx$ and by difference

$$\int_\Omega |\mathcal{E}^D u_h| dx \to \int_\Omega |E^D u|\,.$$

The energy density W^{**} has linear growth in the deviatoric part $\mathcal{E}^D u_h$, and by the continuity statement quoted after (3.7) it follows that

$$\int_\Omega W^{**}(\mathcal{E}^D u_h)dx \to \int_\Omega W^{**}(\mathcal{E}^D u)dx + \int_\Omega W^\infty\left(\frac{E_s u}{|E_s u|}\right) d|E_s u|\,.$$

Combining the two results, we get $J(u_h) \to J(u)$.

Finally, we show that for any $v \in C^\infty$, it is possible to find a sequence v_k converging to v weakly in $W^{1,2}$ such that

$$\int_\Omega W(\nabla v_k)dx \to \int_\Omega W^{\mathrm{qc}}(\nabla v)dx\,, \qquad v_k = v \text{ on } \partial\Omega, \tag{3.10}$$

where W^{qc} is the quasiconvex envelope of W, as defined in (3.3). This follows from the general theory, since the function W is continuous and v is uniformly Lipschitz, see e.g. [38]; for the convenience of the reader we sketch here the argument. By density we can find a sequence of uniformly Lipschitz, piecewise affine functions w_k which converge to v in $W^{1,2}$ and are such that the integral of $W^{\mathrm{qc}}(\nabla w_k)$ converges to the integral of $W^{\mathrm{qc}}(\nabla v)$. Fix a sequence $\varepsilon_k \to 0$, $\varepsilon_k > 0$, and consider one k. Let ω be one of the parts of the domain where w_j is affine, say $w_j = \beta x + c$ on ω. By (3.3) there is u such that $u(x) = \beta x$ on the boundary of the unit cube, and $\int_{(0,1)^3} W(\nabla u)dx \leqq W^{\mathrm{qc}}(\beta) + \varepsilon_k$. The set ω can be covered by finitely many small cubes $(0, l_i)^3 + p_i$, up to a remainder whose measure is less than $\varepsilon|\omega|$. In each such cube we set $v_k(l_i x + p_i) = l_i u(x) + c$, outside the cubes $v_k = w_k$. This gives

$$\begin{aligned}
\int_\omega W(\nabla v_k)dx &= \sum_i \int_{(0,l_i)^3+p_i} W(\nabla v_k)dx + \varepsilon_k|\omega|W(\beta) \\
&\leqq \sum_i l_i^3 \left[W^{\mathrm{qc}}(\beta) + \varepsilon_k\right] + \varepsilon_k|\omega|W(\beta) \\
&\leqq |\omega| W^{\mathrm{qc}}(\beta) + \varepsilon_k|\omega|\,[1 + W(\beta)]\,.
\end{aligned}$$

Summing over all sets ω_j covering Ω, and using the fact that by continuity W is uniformly bounded on the support of the uniformly bounded functions ∇w_k, we get

$$\int_\Omega W(\nabla v_k)dx \leqq \sum_j |\omega_j| W^{\mathrm{qc}}(\beta_j) + \varepsilon_k |\omega_j| \left[1 + W(\beta_j)\right]$$
$$\leqq \int_\Omega W^{\mathrm{qc}}(\nabla v_k)dx + \varepsilon_k |\Omega| \left[1 + M\right] .$$

Taking the $k \to \infty$ limit, we find that the sequence ε_k converges to zero, and the integral of $W^{\mathrm{qc}}(\nabla v_k)$ converges to the integral of $W^{\mathrm{qc}}(\nabla v)$. This concludes the proof of (3.10).

We show in Proposition 3.4 below that the quasiconvex envelope coincides with the convex one, $W^{\mathrm{qc}} = W^{**}$. Taking a diagonal subsequence, the proof is concluded. □

3.4. The quasiconvex envelope

We now compute the quasiconvex envelope of W, defined in (3.3), under the assumption that the set of slip systems is complete, in the sense of Definition 3.2. Our main result is the following

Proposition 3.4. *Let $\mathcal{S}$ be a complete family of slip systems. Then, the quasiconvex envelope of W coincides with the convex one, $W^{\mathrm{qc}} = W^{**}$.*

Before proving the proposition we give some partial results concerning the lamination convex envelope of W. This corresponds to including the energy W in the kinematic considerations of Section 3.2. Precisely, we not only keep track of which average strains can be generated using the available slips, but also of which slips are used, and how much energy they cost.

We recall that a probability measure on 3×3 matrices $\nu = \lambda_1 \delta_{\beta_1} + \lambda_2 \delta_{\beta_2}$ is a first-order laminate with average β if $\lambda_1 \beta_1 + \lambda_2 \beta_2 = \beta$ and $\mathrm{rank}(\beta_1 - \beta_2) = 1$. Here δ_β denotes a Dirac mass supported on the matrix β. Laminates of order k with average β are then defined as the set of probability measures obtained from laminates of order $k-1$ replacing any δ_{β_j} with a first-order laminate with average β_j. Laminates offer a natural way to reduce the energy by using deformation patterns admissible for gradient fields (see, e.g., [38]). We call the union of all laminates of order k for $k \in \mathbb{N}$ laminates of finite order, or briefly, laminates. Note that we do not take the closure, hence all laminates here have finite order. This permits us to avoid subtleties arising from the linear growth.

The assumption of completeness implies that the lamination envelope W^{lc} has linear growth on traceless matrices.

Lemma 3.5. *Let $\mathcal{S}$ be a complete set of slip systems. Then there is a constant c such that for any β there is a laminate ν (of finite order) such that*

$$\beta = \langle \nu, \mathrm{Id} \rangle , \qquad \textit{and} \qquad \langle \nu, W \rangle \leqq c \left(|\beta^{\mathrm{sym}}| + |\operatorname{Tr} \beta|^2 \right) .$$

Proof. Since W only depends on the symmetric part of β, we only need to prove the result for symmetric β. We decompose β as in (3.8), $\beta = \beta^D + p \operatorname{Tr} \beta$, and first consider the plastic part of the potential alone, as a function of the deviatoric part β^D. Since $\mathcal{S}$ is complete, there is $\eta > 0$ such that all traceless matrices of norm less than or equal to η are averages of laminates supported on $\pm\mathcal{S}$. For all such laminates

$$\langle \nu, W \rangle \leqq \max_i \tau_i \,,$$

and the bound is obtained without any elastic energy, hence has linear scaling. In particular, the matrix $\tilde{\beta}^D = (\eta/|\beta^D|)\beta^D$ has such a representation. Call it $\tilde{\nu}^D$. The laminate ν^D is obtained from $\tilde{\nu}^D$ by scaling the support by $|\beta^D|/\eta$. Since the plastic part of the energy is positively homogeneous of degree one, we get

$$\langle \nu^D, W \rangle \leqq \frac{|\beta^D|}{\eta} \max_i \tau_i = c|\beta^D| \leqq c|\beta^{\mathrm{sym}}|.$$

The laminate ν is obtained from ν^D by translating its support by the volumetric part $p \operatorname{Tr} \beta$. Since $W(p \operatorname{Tr} \beta + \beta^D) \leqq c|\operatorname{Tr} \beta|^2 + W(\beta^D)$ we obtain the thesis. □

Lemma 3.6. *Let $\mathcal{S}$ be a complete set of slip systems. For any $\beta \in \mathbb{R}^{3\times 3}$ and any $\varepsilon > 0$ there is a laminate ν (of finite order) such that*

$$\langle \nu, \mathrm{Id} \rangle = \beta \qquad \textit{and} \qquad \langle \nu, W \rangle \leqq W^{**}(\beta) + \varepsilon \,.$$

Proof. By Lemma 3.1(i) we can find $\gamma \in \mathbb{R}^N$, a symmetric ϵ^e, and a skew-symmetric ω such that

$$\beta = \epsilon^e + \sum_{i=1}^{k} \gamma_i s_i \otimes m_i + \omega \qquad \text{and} \qquad W^{**}(\beta) = \frac{1}{2}(C\epsilon^e, \epsilon^e) + \sum_{i=1}^{k} \tau_i \gamma_i$$

for some $k \leqq N$. We now prove the thesis by induction on k. The cases $k = 0$ and $k = 1$ are trivial. Assume now that the thesis holds for $k - 1$, and let

$$\beta_1 = \epsilon^e + \sum_{i=1}^{k-1} \gamma_i s_i \otimes m_i + \omega \qquad \text{and} \qquad \beta_2 = \beta_1 + \frac{1}{\varepsilon}\gamma_k s_k \otimes m_k \,.$$

They are clearly rank-one connected. The matrix β is the average of a laminate supported on β_1 and β_2, with weights $1 - \varepsilon$ and ε respectively. At the same time, β_2 is the average of a laminate supported on

$$\beta_3 = \epsilon^e + \sum_{i=2}^{k-1} \gamma_i s_i \otimes m_i + \frac{1}{\varepsilon}\gamma_k s_k \otimes m_k + \omega \,, \quad \text{and} \quad \beta_4 = \beta_3 + \frac{1}{\varepsilon}\gamma_1 s_1 \otimes m_1 \,,$$

again with weights $1 - \varepsilon$ and ε (here the lamination direction $s_1 \otimes m_1$ has been used). Note that the sum in the definition on β_3 starts from $i = 2$, hence β_3 is the

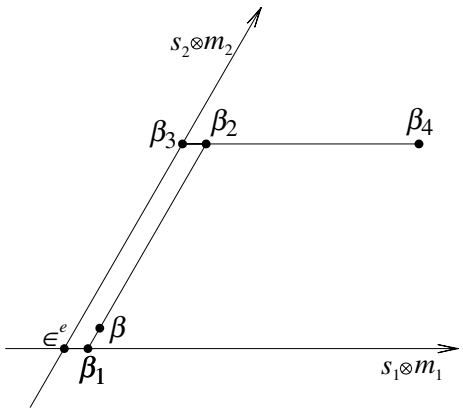


Fig. 3.1. Construction used in proving Lemma 3.6, in the case $k = 2$ of two slip systems. The arrows indicate the rank-one directions $s_1 \otimes m_1$ and $s_2 \otimes m_2$.

sum of $k - 1$ single slips (the summation is understood to be empty if $k = 2$). Combining the two, we obtain a laminate

$$\nu = (1-\varepsilon)\delta_{\beta_1} + \varepsilon(1-\varepsilon)\delta_{\beta_3} + \varepsilon^2\delta_{\beta_4}$$

with average β. By the inductive assumption, β_1 and β_3 can be generated as laminates with energies controlled by $W^{\mathrm{qc}}(\beta_1) + \varepsilon$ and $W^{\mathrm{qc}}(\beta_3) + \varepsilon$ respectively, and by Lemma 3.5 there is a laminate ν_4 such that

$$\langle \nu_4, \mathrm{Id}\rangle = \beta_4\,, \qquad \langle \nu_4, W\rangle \leqq c\left(|\beta_4^{\mathrm{sym}}| + |\operatorname{Tr}\beta_4|^2\right) \leqq c\frac{|\beta^{\mathrm{sym}}|}{\varepsilon} + c|\operatorname{Tr}\beta|^2\,.$$

We conclude that there is a laminate with average β and energy controlled by

$$\begin{aligned}\langle \nu, W\rangle &\leqq (1-\varepsilon)W(\beta_1) + \varepsilon W(\beta_3) + c\varepsilon|\beta^{\mathrm{sym}}| + c\varepsilon^2|\operatorname{Tr}\beta|^2 + \varepsilon \\ &\leqq \frac{1}{2}(C\epsilon^e, \epsilon^e) + \sum_{i=1}^{k}\tau_i\gamma_i + c(\beta^{\mathrm{sym}})\varepsilon\,,\end{aligned}$$

where the last constant depends on β^{sym} but not on ε. This concludes the proof. □

Proposition 3.4 is then an easy consequence.

Proof of Proposition 3.4. The quasiconvex envelope is larger than or equal to the convex one, hence the result is established if we can show that for any $\beta \in \mathbb{R}^{3\times 3}$ and $\varepsilon > 0$, there is a function $u \in W^{1,\infty}((0,1)^3, \mathbb{R}^3)$ such that

$$\int_{(0,1)^3} W(\nabla u)dx \leqq W^{**}(\beta) + \varepsilon\,, \qquad u(x) = \beta x \quad \text{if } x \in \partial(0,1)^3\,.$$

Consider the laminate ν obtained in Lemma 3.6. It is a laminate of finite order, supported on a bounded subset of $\mathbb{R}^{3\times 3}$. Then, we can find a sequence u_h of uniformly Lipschitz functions which coincide with βx on the boundary and are such that $\nabla u_h \rightharpoonup \nu$, in the sense of Young measures [38]. In particular, since W is continuous for large enough h, we get

$$\int_{(0,1)^3} W(\nabla u_h) dx \leqq \langle \nu, W\rangle + \varepsilon \leqq W^{**}(\beta) + 2\varepsilon\,.$$

This concludes the proof. □

3.5. Completeness of the fcc and bcc slip systems

We now show that the slip systems appearing in fcc and bcc crystals are complete, in the sense of Definition 3.2. To do this, for any traceless β we construct a laminate with average β supported on a multiple of $\pm\mathcal{S}$. These constructions need not be, and are not, optimal from the point of view of the energy, since they are only used in the error term (the part called β_4 in the proof of Lemma 3.6). The optimal energy scaling is then recovered with the argument discussed above and illustrated in Fig. 3.1.

Lemma 3.7. *The set of fcc slip systems $\mathcal{S}_{\rm fcc}$, containing all symmetry-related copies of the pair $s = (1, 1, 0)$, $m = (1, -1, 1)$ as given in Table 2.1, is complete.*

Proof. We need to show that all small enough symmetric traceless matrices are averages of laminates supported on $\pm\mathcal{S}_{\rm fcc}$, modulo rotations. The set $\pm\mathcal{S}_{\rm fcc}$ is invariant under the following symmetry operations (which stem from the cubic group of the fcc crystal): (i) changing the global sign; (ii) interchanging the i-th and j-th row and *at the same time* the i-th and j-th column; (iii) changing sign to the i-th row and *at the same time* to the i-th column. Therefore all results are invariant under those symmetry operations. Further, we can identify matrices which have the same symmetric part, since rotations are irrelevant, and multiply each matrix by a positive number, by scaling.

Step 1. All matrices of the form

$$\beta_{a,b} = \begin{pmatrix} a & b & 0 \\ b & -a & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and equivalent can be generated. Since all matrices of this form have zero determinant, all linear combinations in this class are permissible. Therefore it is sufficient to prove the result assuming that only one between a and b is nonzero. We do this separately in the two cases.

Case $b = 0$: Consider the two slip systems with $s = s_1 = (1, 1, 0)$, which have $m_1^a = (1, -1, 1)$ and $m_1^b = (1, -1, -1)$. Since s is the same, any linear combination between them can be obtained by a laminate, in particular $[s_1 \otimes (m_1^a + m_1^b)/2]^{\rm sym} = e_1 \otimes e_1 - e_2 \otimes e_2 = \beta_{1,0}$ can be obtained as a laminate, and by scaling all $\beta_{a,0}$.

Case $a = 0$: Start from the two slip systems with $s = s_2 = (1, 0, 1)$, which have $m_2^a = (1, 1, -1)$ and $m_2^b = (1, -1, -1)$. They generate the matrix $\bar{\beta} = s_2 \otimes (m_2^a - m_2^b)/2 = s_2 \otimes e_2$. The same argument starting from $s_2' = (1, 0, -1)$ leads to the matrix $\bar{\beta}' = s_2' \otimes e_2$. The two matrices $\bar{\beta}$ and $\bar{\beta}'$ are rank-one connected, and therefore their average $(\bar{\beta} + \bar{\beta}')/2 = e_1 \otimes e_2$ can be generated as a laminate. Taking the symmetric part and scaling we then obtain all $\beta_{0,b}$. This concludes the proof of Step 1.

Step 2. All matrices of the form

$$\beta_1 = \begin{pmatrix} a & b & 0 \\ b & -a-c & d \\ 0 & d & c \end{pmatrix}$$

with $a \geqq c > 0$ and equivalent can be generated as laminates. We start from the two matrices

$$\beta_2 = \begin{pmatrix} a & b & 0 \\ b & -a & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \beta_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -c & d \\ 0 & d & c \end{pmatrix}$$

which can be generated by Step 1, and observe that

$$\det(\beta_2 - \lambda\beta_3) = c(a^2 + b^2)\lambda - a(c^2 + d^2)\lambda^2$$

vanishes for $\lambda = 0$ and $\lambda = \bar{\lambda} > 0$. Therefore all linear combinations with coefficents of the same sign, including $\beta_1 = \beta_2 + \beta_3$, can be generated.

Step 3. We finally show that each traceless matrix can be generated. It is sufficient to consider matrices of the form

$$\beta = \begin{pmatrix} a' & b & f \\ b & -a'-c' & d \\ f & d & c' \end{pmatrix},$$

where $a' \geqq c' \geqq 0$ (two of the diagonal entries always have the same sign, indices can be permuted, and the global sign can be changed). Fix some e and define

$$\beta_4 = \begin{pmatrix} e & 0 & f \\ 0 & 0 & 0 \\ f & 0 & -e \end{pmatrix},$$

which can be generated as a laminate by Step 1, and β_1 as in Step 2, with $a = a' - e$, $c = c' + e$, so that $\beta = \beta_1 + \beta_4$. If $a' > 0$, choosing $e = a'/2$ we can have $a > 0$, $c > 0$, hence β_1 can be generated as a laminate by Step 3. Consider now

$$\begin{aligned} \det(\beta_1 - \lambda\beta_4) = &-\Big[c(a^2 + b^2) + a(c^2 + d^2)\Big] \\ &+\Big[e(c^2 + d^2 - a^2 - b^2) - 2bdf\Big]\lambda + (a + c)(e^2 + f^2)\lambda^2 . \end{aligned}$$

This has two nonvanishing zeroes in λ, one positive and the other negative. Choosing the positive one, we obtain a rank-one connection between β_1 and a positive multiple of β_4, which, after scaling, can generate $\beta = \beta_1 + \beta_4$.

It remains to consider the case $a' = c' = 0$, where the matrix β is purely off-diagonal. But this is a direct consequence of the case $a' > 0$, since

$$\begin{pmatrix} 0 & b & f \\ b & 0 & d \\ f & d & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & b & f \\ b & -1 & d \\ f & d & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} -1 & b & f \\ b & 1 & d \\ f & d & 0 \end{pmatrix}$$

and the difference of the two matrices has zero determinant. This concludes the proof. □

Lemma 3.8. *Each of the two sets of bcc slip systems, as given in Table 2.2, is complete.*

Proof. The first set of slip systems is obtained from the one of fcc by transposition, and since only the symmetric part is relevant in computing symmetric lamination envelopes, its completeness follows from Lemma 3.7. Consider now the second one. Take $s = s_1 = (1, 1, 1)$, $m = m_{1a} = (-2, 1, 1)$ and $m_{1b} = (1, -2, 1)$. These two slip systems are rank-one connected, since s is the same. On the other hand, $m_{1a} - m_{1b} = (-3, 3, 0)$. Due to the cubic symmetry, this suffices to prove that all slips in the first set are generated as averages of slips in the second one. Therefore the latter is also complete. □

It would be tempting to conjecture that all slip systems which span the set of traceless matrices are complete. This is, however, not true, as we now show with an explicit example.

Lemma 3.9. *Consider the set of slip systems*

$$\mathcal{S}_* = \{e_1 \otimes e_2,\ e_1 \otimes e_3,\ (e_1 + e_2) \otimes (e_1 - e_2),\ (e_1 + e_3) \otimes (e_1 - e_3),\\ (e_1 + e_2 + e_3) \otimes (2e_1 - e_2 - e_3)\}\ .$$

The symmetric parts of the matrices in $\mathcal{S}_*$ span the set of symmetric traceless matrices, but $\mathcal{S}_*$ is not complete.

Proof. We first observe that each pair (s, m) is composed of two orthogonal vectors, each pair (s, m) spans a space which contains e_1, and the set of matrices $(s \otimes m)^{\mathrm{sym}}$ are five linearly independent traceless symmetric matrices, hence span the space of symmetric traceless matrices.

We now show that $\mathcal{S}$ is not complete. We reason by contradiction, and assume that for some small $\eta > 0$ there is a laminate supported on $\pm\mathcal{S}_* + so(3)$ with average $\beta = \eta(e_2 \otimes e_3)^{\mathrm{sym}}$. Then for any $\varepsilon > 0$, there is a function $u : (0, 1)^3 \to \mathbb{R}^3$ such that $u(x) = \beta x$ on the boundary, $|\nabla u| \leqq M$, and $\nabla u^{\mathrm{sym}} \in \pm\mathcal{S}_*^{\mathrm{sym}}$ away from a set ω of measure ε. Here M depends only on the laminate, not on ε or u. Since the cofactor of a gradient is a divergence, its integral depends only on the boundary values, and in particular

$$\int_{(0,1)^3} \operatorname{cof} \nabla u \, dx = \operatorname{cof} \beta = -\eta^2 e_1 \otimes e_1\,. \tag{3.11}$$

On the other hand, away from the small set ω,

$$\nabla u = \pm s \otimes m + \omega_a$$

for some (x-dependent) $\omega_a \in so(3)$ and $s \otimes m \in \mathcal{S}_*$. We parametrize here antisymmetric matrices by their axial vector a, defined by $\omega_a v = v \wedge a$ for all $v \in \mathbb{R}^3$. A straightforward computation shows that

$$\operatorname{cof}(\pm s \otimes m + \omega_a) = a \otimes a \pm a \otimes (s \wedge m) \pm (s \cdot a)\omega_m,$$

where the last term contains the antisymmetric matrix with axial vector m. Taking the 11 component, we get

$$e_1 \cdot \operatorname{cof}(\pm s \otimes m + \omega_a) e_1 = (a \cdot e_1)^2$$

since ω_m is antisymmetric, and $s \wedge m$ is orthogonal to e_1 (here we use the fact that all pairs (s, m) span a space containing e_1). Comparing with (3.11) we get

$$-\eta^2 = e_1 \cdot \int_{(0,1)^3} \operatorname{cof} \nabla u \, dx \cdot e_1 \geqq \int_{(0,1)^3} (a \cdot e_1)^2 dx - M^2 \varepsilon$$

for any $\varepsilon > 0$. This implies $-\eta^2 \geqq 0$, a contradiction. □

In closing, we remark that many average deformations can be obtained with specific constructions that require less surface energy. This is irrelevant for the purpose of determining the relaxation of the energy, but makes a difference if higher-order corrections (nonlocal terms) are included. The next section presents a characterization of the minimal complexity of the microstructure required to relax the energy for some simple average strains.

3.6. Slip concentration

In computing the quasiconvex envelope of W in Section 3.5 we made use of a construction which contains very large strains on parts of the domain, which converge to slip lines in the limit. We investigate now whether such slip lines are necessary in order to obtain the optimal energy, or if instead a different construction with bounded strains is always possible. In particular, we focus on the fcc set of slip systems and on the case of plastic deformations which are a linear combination of two slips,

$$\beta^p = \alpha_1 s_1 \otimes m_1 + \alpha_2 s_2 \otimes m_2, \qquad (s_1, m_1) \text{ and } (s_2, m_2) \in \mathcal{S}_{\text{fcc}},$$

for some $\alpha_1, \alpha_2 \neq 0$. We shall show that for some such average strains a simple first-order laminate permits us to realize the optimal energy. For other choices instead no structure with bounded gradients realizes the optimal energy, and strain necessarily concentrates, at least in an L^2 sense. This is an indication that concentrated slip (slip lines) is necessary to fully relax the energy.

We start with the positive case. Following ORTIZ & REPETTO [42] we have

Lemma 3.10. *Let (s_1, m_1) and (s_2, m_2) be two slip systems. Then, there is a simple laminate such that the strain is supported on*

$$r_1(s_1 \otimes m_1)^{\mathrm{sym}} \qquad r_2(s_2 \otimes m_2)^{\mathrm{sym}}$$

with $r_1, r_2 \neq 0$ if and only if

$$r_2(t_2 \cdot s_1)(t_2 \cdot m_1) = r_1(t_1 \cdot s_2)(t_1 \cdot m_2)\,,$$

where $t_i = s_i \wedge m_i$.

Proof. Let $\epsilon_i = r_i(s_i \otimes m_i)^{\mathrm{sym}}$ denote the corresponding strains. Based on the discussion in Section 3.2, it suffices to check if the traceless matrix $\epsilon_1 - \epsilon_2$ is singular, i.e., if

$$0 = \det(\epsilon_1 - \epsilon_2) = \epsilon_1 : \operatorname{cof} \epsilon_2 - \epsilon_2 : \operatorname{cof} \epsilon_1$$

since $\det \epsilon_1 = \det \epsilon_2 = 0$. Here, $A : B = \operatorname{Tr} A^T B = A_{ij} B_{ij}$. Since $\operatorname{cof}[(r_i s_i \otimes m_i)^{\mathrm{sym}}] = r_i^2 t_i \otimes t_i$, the thesis follows. □

In particular, Lemma 3.10 shows that if the sign condition

$$\alpha_1\alpha_2(t_2 \cdot s_1)(t_2 \cdot m_1)(t_1 \cdot s_2)(t_1 \cdot m_2) \geqq 0$$

holds, then there is a simple laminate between matrices of the form

$$\beta_1 = r_1 s_1 \otimes m_1 + \omega_1 \qquad \text{and} \qquad \beta_1 = r_2 s_2 \otimes m_2 + \omega_2$$

with average $\beta^p = \alpha_1 s_1 \otimes m_1 + \alpha_2 s_2 \otimes m_2$ (the weights are constructed as in Section 3.1).

We now show that the condition above for the existence of a simple laminate between two slip systems is actually necessary for the existence of a polyconvex measure supported on the two independent slip systems. By independent we mean that the symmetrized shears $(s \otimes m)^{\mathrm{sym}}$ and $(s' \otimes m')^{\mathrm{sym}}$ are linearly independent in $\mathbb{R}^{3\times 3}$. We shall then in Proposition 3.12 discuss the general case, where only the average strain is prescribed.

Lemma 3.11. *Let (s_1, m_1) and (s_2, m_2) be two independent slip systems, and fix two orientations $\sigma_i \in \{\pm 1\}$. If*

$$\sigma_1\sigma_2(t_2 \cdot s_1)(t_2 \cdot m_1)(t_1 \cdot s_2)(t_1 \cdot m_2) < 0, \tag{3.12}$$

then any L^2 polyconvex measure supported on the union of the two sets

$$\mathcal{G}_i = \left\{\beta \in \mathbb{R}^{3\times 3} : \beta^{\mathrm{sym}} = \lambda\sigma_i(s_i \otimes m_i)^{\mathrm{sym}}\,,\ \ \lambda \geqq 0\right\}$$

(for $i \in \{1, 2\}$) is actually supported on one of them.

Proof. Consider an L^2 polyconvex measure supported on $\mathcal{G}_1 \cup \mathcal{G}_2$, i.e., a probability measure ν on $\mathbb{R}^{3\times 3}$ which obeys the conditions

$$\beta = \langle \nu, \mathrm{Id} \rangle , \qquad \mathrm{cof}\, \beta = \langle \nu, \mathrm{cof} \rangle . \tag{3.13}$$

Note that the assumption that ν is an L^2 Young measure permits us to compute the average of the cofactor, which is a quadratic quantity, but not that of the determinant, which is cubic. The first of the (3.13) gives

$$\beta = \lambda_1 \sigma_1 s_1 \otimes m_1 + \lambda_2 \sigma_2 s_2 \otimes m_2 + \omega ,$$

where $\omega \in so(3)$ and $\lambda_{1,2} \geqq 0$. We assume without loss of generality that $\omega = 0$. Since the slip systems are independent, if one of the λ_i's vanishes the thesis is proved. From now on we assume that both are strictly positive and show that this leads to a contradiction. The proof proceeds in strict analogy with the argument of Lemma 3.9. Precisely, we compute the cofactor of β,

$$\mathrm{cof}\, \beta = \lambda_1 \lambda_2 \sigma_1 \sigma_2 (s_1 \wedge s_2) \otimes (m_1 \wedge m_2) .$$

With the definition $v = t_1 \wedge t_2$, where as above $t_i = s_i \wedge m_i$, (3.12) is equivalent to

$$v \cdot (\mathrm{cof}\, \beta) v < 0 \tag{3.14}$$

(again, this is a simple expansion based on the usual manipulation rules for wedge products). On the other hand, for any Young measure supported on $\mathcal{G}_1 \cup \mathcal{G}_2$, the expression $v(\mathrm{cof}\, \cdot)v$ has nonnegative average. Indeed, if $G \in \mathcal{G}_i$, then $G = \omega_a + \lambda \sigma_i s_i \otimes m_i$, for some $\lambda \geqq 0$ and skew-symmetric ω_a (parametrized as in Lemma 3.9 by its axial vector a), and

$$\mathrm{cof}(\omega_a + \sigma s \otimes m) = a \otimes a + \sigma a \otimes (s \wedge m) + \sigma (s \cdot a) \omega_m .$$

We obtain, for any $G \in \mathcal{G}_1 \cup \mathcal{G}_2$,

$$v(\mathrm{cof}\, G) v = v\, \mathrm{cof}(\omega_a + \lambda \sigma_i s_i \otimes m_i) v = (a \cdot v)^2 \geqq 0$$

since v is orthogonal to both t_1 and t_2, and ω_a is antisymmetric. A comparison with the second equation in (3.13) and (3.14) concludes the proof. □

The above result assumes that only two slip systems are used. We now show that for some average strains β no construction with bounded strains, and in particular no laminate of finite order, achieves the optimal energy.

Proposition 3.12. *Consider the fcc set of slip systems $\mathcal{S}_{\mathrm{fcc}}$ and a positive-definite elasticity matrix C. Then there is a strain β with the following property. For any $u \in W^{1,2}$ such that*

$$\frac{1}{\Omega} \int_\Omega |\nabla u|^2 dx \leqq M \qquad \textit{and} \qquad u(x) = \beta x \textit{ on } \partial\Omega ,$$

where Ω is a Lipschitz domain, the following inequality holds:

$$\frac{1}{\Omega} \int_\Omega W(\nabla u) dx \geqq W^{\mathrm{qc}}(\beta) + c(M) ,$$

where $c(M)$ is a positive constant which only depends on M, not on u.

Proof. The proof is by contradiction. If the thesis were false, there would be for some $M > 0$ a sequence u_h such that

$$\frac{1}{\Omega}\|\nabla u_h\|^2_{L^2(\Omega)} \leqq M\,, \quad u_h(x) = \beta x \text{ on } \partial\Omega\,, \quad \frac{1}{\Omega}\int_\Omega W(\nabla u_h)dx \to W^{\mathrm{qc}}(\beta)\,.$$

The sequence ∇u_h generates in the limit an L^2 Young measure, and by a standard scaling and covering argument we can assume it to be homogeneous. Since it originates from a sequence of gradients, it is a polyconvex measure, and satisfies

$$\langle \nu, \mathrm{Id}\rangle = \beta\,, \qquad \langle \nu, \mathrm{cof}\rangle = \mathrm{cof}\,\beta\,, \qquad \langle \nu, W\rangle = W^{**}(\beta)\,.$$

We now intend to use Lemma 3.11 to show that for suitable choices of β these three conditions are incompatible with each other. In order to do this, we start by constructing a linear lower bound for W which is equal to W only on β and on two slip systems, and therefore proves that only two slip systems can be used by ν.

Consider the scalar product $\langle\cdot,\cdot\rangle_*$ defined on $\mathbb{R}^{3\times3}$ by

$$\langle \beta, \beta'\rangle_* = \sum_{i\neq j}\beta_{ij}\beta'_{ij} + \frac{1}{6}\sum_i \beta_{ii}\beta'_{ii}\,.$$

The matrices $M_i = (s_i \otimes m_i)^{\mathrm{sym}}$ characterizing the symmetrized individual slips have the products

$$\langle M_i, M_i\rangle_* = \frac{4}{3}\,, \qquad \langle M_i, M_j\rangle_* \in \left\{\pm\frac{1}{3}, \pm\frac{2}{3}\right\} \text{ if } i \neq j$$

(to see this, it is sufficient to compute explicitly a few not symmetry-related cases; for brevity we do not report the full details here). Now consider for $s \in \{\pm1\}$ the linear map defined on $\mathbb{R}^{3\times3}$ by

$$f(\beta) = \langle M_1 + sM_2, \beta\rangle_*\,.$$

Here, M_1 and M_2 correspond to the first two entries in $\mathcal{S}_{\mathrm{fcc}}$, which are any pair of fcc slip systems. For simplicity of notation we denote them by 1 and 2. It is clear that

$$f(M_1) = f(sM_2) = \langle M_1, M_1\rangle_* + s\langle M_1, M_2\rangle_*\,.$$

Choose $s \in \{\pm1\}$ to have the same sign as $\langle M_1, M_2\rangle_*$. Then both terms in the expression above are positive. We define H by

$$f(M_1) = f(sM_2) = H \geqq \tfrac{5}{3}\,.$$

On the other hand, if $i \geqq 3$, we have

$$f(\pm M_i) = \pm\langle M_1, M_i\rangle_* \pm s\langle M_2, M_i\rangle_* \leqq \tfrac{4}{3} < H\,.$$

Now let $\sigma_0 \in \mathbb{R}^{3\times 3}$ be a symmetric matrix defined by

$$(\sigma_0, \beta) = \frac{\tau}{H} f(\beta^{\mathrm{sym}}) \qquad \text{for all } \beta \in \mathbb{R}^{3\times 3}$$

and $\beta_0^e = C^{-1}\sigma_0$. We claim that, for any β,

$$W^{**}(\beta) \geqq \frac{\tau}{H} f(\beta - \beta_0) + W^{**}(\beta_0), \tag{3.15}$$

where

$$\beta_0 = \beta_0^e + \beta_0^p\,, \qquad \beta_0^p = \beta^p(\gamma^0) = M_1 + sM_2\,.$$

Here and below, $\gamma_1^0 = 1$, $\gamma_2^0 = s$, and $\gamma_i^0 = 0$ for $i \geqq 3$. To prove (3.15), we compute (with the usual notation $\epsilon^e = (\beta - \beta^p(\gamma))^{\mathrm{sym}}$, $\epsilon_0^e = (\beta_0^e)^{\mathrm{sym}}$, etc.)

$$\begin{aligned}
A(\beta,\gamma) &= \frac{1}{2}(C\epsilon^e, \epsilon^e) + \tau \sum |\gamma_i| \\
&= \frac{1}{2}\left(C(\epsilon^e - \epsilon_0^e), (\epsilon^e - \epsilon_0^e)\right) + (C\epsilon_0^e, \epsilon^e - \epsilon_0^e) + \frac{1}{2}(C\epsilon_0^e, \epsilon_0^e) + \tau \sum |\gamma_i| \\
&\geqq c|\epsilon^e - \epsilon_0^e|^2 + \frac{\tau}{H} f(\epsilon^e - \epsilon_0^e) + \frac{1}{2}(C\epsilon_0^e, \epsilon_0^e) + \tau \sum |\gamma_i| \\
&\geqq c|\epsilon^e - \epsilon_0^e|^2 + \frac{\tau}{H} f(\epsilon - \epsilon_0) \\
&\quad + \frac{\tau}{H} f(\epsilon_0^p - \epsilon^p) + \frac{1}{2}(C\epsilon_0^e, \epsilon_0^e) + \tau \sum |\gamma_i|\,.
\end{aligned}$$

Now we focus on the two terms depending only on the plastic part. Since by construction $f(M_1)/H = \gamma_1^0 = 1$, $f(M_2)/H = \gamma_2^0 = s$, and for $i \geqq 3$ we have $f(M_i)/H < 1$ and $\gamma_i^0 = 0$, we get

$$\frac{\tau}{H} f(\epsilon_0^p - \epsilon^p) + \tau \sum_i |\gamma_i| = \tau \sum_i \left[|\gamma_i| + \frac{f(M_i)}{H}(\gamma_i^0 - \gamma_i) \right] \geqq \tau \sum_i |\gamma_i^0|\,.$$

Equality here holds only if $\gamma_1 \geqq 0$, $s\gamma_2 \geqq 0$, and $\gamma_i = 0$ for $i \geqq 3$. We conclude that

$$A(\beta,\gamma) \geqq A(\beta_0, \gamma^0) + \frac{\tau}{H} f(\beta - \beta_0)$$

for all β and γ. Taking the minimum over γ we get (3.15), with equality holding only if $\epsilon^e = \epsilon_0^e$, $\gamma_1 \geqq 0$, $s\gamma_2 \geqq 0$, and $\gamma_i = 0$ for $i \geqq 3$. Therefore both conditions must hold ν-almost everywhere. This implies that the Young measure μ obtained translating ν by $-\epsilon_0^e$ is supported on the set

$$\mathcal{G}_1^1 \bigcup \mathcal{G}_2^s,$$

where

$$\mathcal{G}_i^t = \left\{ F : F^{\mathrm{sym}} = \lambda t (s_i \otimes m_i)^{\mathrm{sym}}\,, \lambda \geqq 0 \right\}$$

and has average $\beta_0^p = M_1 + sM_2$. If the sign condition (3.12) holds, by Lemma 3.11 the measure μ is actually supported on one of them, but this contradicts the fact that the average is the sum of two (linearly independent) slips. We finally check that there are pairs of slip systems which obey (3.12). To do this, we need to find (s_1, m_1) and (s_2, m_2) in $\mathcal{S}_{\text{fcc}}$, $s \in \{\pm 1\}$, such that

$$s(t_2 \cdot s_1)(t_2 \cdot m_1)(t_1 \cdot s_2)(t_1 \cdot m_2) < 0\,,$$

where s has the same sign as $\langle (s_1 \otimes m_1)^{\text{sym}}, (s_2 \otimes m_2)^{\text{sym}} \rangle_*$. One such pair is

$$s_1 = (-1, 0, 1)\,, \qquad m_1 = (1, -1, 1)\,, \qquad s_2 = (1, -1, 0)\,, \qquad m_2 = (1, 1, 1)\,,$$

with the same orientation (i.e., $s = 1$); by symmetry there are 11 other equivalent pairs. Indeed, a simple computation shows that $t_1 = (1, 2, 1)$, $t_2 = (-1, -1, 2)$, and $(t_2 \cdot s_1)(t_2 \cdot m_1)(t_1 \cdot s_2)(t_1 \cdot m_2) = -24$. On the other hand, the scalar product is $\langle (s_1 \otimes m_1)^{\text{sym}}, (s_2 \otimes m_2)^{\text{sym}} \rangle_* = 1/3 > 0$. This concludes the proof. □

We conclude that, given any pair of slip systems, it is possible to find a lamination between them, but the same is not true if the orientation is prescribed. This implies that in simple tests which activate a linear combination of two slip systems, we expect either a laminate or a more complex pattern involving slip concentration, depending on the relative orientation.

3.7. Inclusion of Dirichlet boundary conditions

We now extend the relaxation result of Section 3.3 to the case where Dirichlet boundary conditions are imposed on part of the boundary. We consider the functional $I(u)$ as defined in (3.1), with additional smoothness imposed on Ω (see the statement of the theorem). The main difficulty here is that slip can concentrate along the boundary. Indeed, only the boundary condition on the component normal to the boundary will survive the relaxation. A jump in the tangential component is instead permitted, and only energetically penalized through the singular part W^∞ of the energy. We denote by $I(u, \Omega)$ the integral of $W(\nabla u)$ on Ω, and by $I_\Gamma(u, \Omega)$ the functional with Dirichlet boundary conditions on $\Gamma \subset \partial\Omega$. Analogously for J.

Theorem 3.13. *Let $I_\Gamma(u, \Omega)$ be as in* (3.1)*, where W was defined in* (2.1) *with a positive-definite elasticity matrix C, and a complete set of slip systems $\mathcal{S}$, and $u_0 \in H^{1/2}(\Gamma)$. Also assume that Ω is an open, bounded, connected set with C^2 boundary, that $\Gamma = \tilde{\Omega} \cap \partial\Omega$, where $\tilde{\Omega}$ is a Lipschitz open set. Then, the relaxation of $I_\Gamma(u, \Omega)$ with respect to strong L^1 convergence is given by*

$$J_\Gamma(u, \Omega) = \begin{cases} \displaystyle\int_\Omega W^{**}(\mathcal{E}u)dx + \int_\Omega W^\infty\left(\frac{E_s u}{|E_s u|}\right) d|E_s u| \\ \qquad \displaystyle + \int_\Gamma W^\infty((u - u_0) \otimes \nu) d\mathcal{H}^2 \\ \qquad\qquad \text{if } u \in U(\Omega) \text{ and } \nu \cdot (u - u_0) = 0 \text{ on } \Gamma, \\ \infty \qquad\qquad\qquad\qquad\qquad\qquad \text{else.} \end{cases}$$

Here, W^{**} and W^{∞} are as in Theorem 3.3, ν is the normal to Γ, and the values of u and u_0 on Γ are intended in the sense of traces.

We use here and below the fact that functions in BD have a trace in $L^1(\partial\Omega)$, see, e.g., [53, 2].

The idea of the proof can be explained with a standard one-dimensional example (see, e.g., [53]). Minimize $\int_0^1 |u_x| dx$, subject to $\int_0^1 u\, dx = 1, u(0) = u(1) = 0$. Minimizing sequences converge to $u(x) = 1$, with energy converging to the limit value 2 – but, if the integrals are interpreted in the usual way, the limit violates the boundary condition and its energy is zero. The simplest way to resolve the problem is to impose boundary conditions not on the *inner* trace, but on the *outer* one. In other words, we extend u to $(-\delta, 1+\delta)$, and impose $u(x) = 0$ for $x < 0$ and $x > 1$. Then, the minimizing sequence converges to the characteristic function of $(0, 1)$, which has two singular contributions to the energy at the endpoints. In our case, two additional difficulties appear: one is that we impose boundary conditions only on part of the boundary, the other is that the trace of Eu has stronger coercivity than the deviatoric part, hence the normal and tangential components have to be treated differently.

We start with compactness.

Lemma 3.14. *Let u_h be a sequence in $W^{1,2}(\Omega, \mathbb{R}^3)$ such that $I_\Gamma(u_j, \Omega) \leqq c$. Then, there is $u \in U(\Omega)$ and a subsequence such that*

$$u_h \to u \text{ strongly in } L^1\,, \qquad Eu_h \rightharpoonup Eu \text{ weakly in } \mathcal{M}\,,$$

$$\operatorname{div} u_h \rightharpoonup \operatorname{div} u \text{ weakly in } L^2\,.$$

Further, if $u_h = u_0$ on $\Gamma \subset \partial\Omega$, then the limit u satisfies $(u - u_0) \cdot \nu = 0$ on Γ.

Proof. The existence of a converging subsequence follows from the compactness result for BD. To prove that the boundary condition is preserved, we observe that the trace of BD functions satisfies Green's formula

$$\int_\Omega (u_h \otimes \nabla\phi)^{\mathrm{sym}} dx + \int_\Omega \phi\; dEu_h = \int_{\partial\Omega} \phi (u_h \otimes \nu)^{\mathrm{sym}} d\mathcal{H}^2$$

for any $\phi \in C^1(\bar{\Omega})$ (see, e.g., [53, Theorem 1.1]). Taking the trace, we get

$$\int_\Omega (u_h \cdot \nabla\phi + \phi \operatorname{div} u_h)\; dx = \int_{\partial\Omega} \phi\; u_h \cdot \nu\, d\mathcal{H}^2\,.$$

Since $u_h \to u$ in L^1 and $\operatorname{div} u_h \to \operatorname{div} u$ weakly in L^2, we obtain, for all such ϕ,

$$\int_{\partial\Omega} \phi\; u_h \cdot \nu\; d\mathcal{H}^2 \to \int_{\partial\Omega} \phi\; u \cdot \nu\; d\mathcal{H}^2\,.$$

By assumption $u_h \cdot \nu = u_0 \cdot \nu$ on Γ for all h, and therefore the same holds for u. □

Now we give a proof of Theorem 3.13.

Proof of Theorem 3.13. We start from the lower bound. Consider a sequence

$$u_h \to u \text{ in } L^1\,, \qquad u_h = u_0 \text{ on } \Gamma\,, \qquad \lim_{h\to\infty} I(u_h, \Omega) = E < \infty\,.$$

As discussed above, we modify the boundary conditions so that they involve the outer trace. To do this, we first extend $u_0 \in H^{1/2}(\Gamma, \mathbb{R}^3)$ to $u_0 \in W^{1,2}(\mathbb{R}^3, \mathbb{R}^3)$. For each u, we define $u^* : \Omega \cup \tilde{\Omega} \to \mathbb{R}^3$ by

$$u^*(x) = \begin{cases} u(x) & \text{if } x \in \Omega, \\ u_0(x) & \text{if } x \in \tilde{\Omega} \setminus \Omega\,. \end{cases}$$

If $u \in W^{1,2}(\Omega)$ and satisfies the boundary condition, then $u^* \in W^{1,2}(\Omega \cup \tilde{\Omega})$. It is also clear that since $u_h \to u$ in $L^1(\Omega)$ we have $u_h^* \to u^*$ in $L^1(\Omega \cup \tilde{\Omega})$.

Given a small $\delta > 0$, let Ω_δ be an open, bounded set such that

$$\Omega \subset \Omega_\delta\,, \qquad \Gamma = \Omega_\delta \cap \partial\Omega\,, \qquad |\Omega_\delta \setminus \Omega| \leqq \delta$$

(such a set can, for example, be defined as the intersection of $\Omega \cup \tilde{\Omega}$ with a neighborhood of Ω). Consider now the sequence $I(u_h^*, \Omega_\delta)$ (no boundary conditions are imposed here). From Theorem 3.3 we get

$$\liminf_{h\to\infty} I(u_h^*, \Omega_\delta) \geqq J(u^*, \Omega_\delta). \tag{3.16}$$

Since outside Ω we have $u_h^* = u^* = u_0 \in W^{1,2}$, Eu_h and Eu^* can have singular contributions only in Ω and on Γ. At the same time, the outer trace on Γ of u^* equals u_0. Therefore (3.16) gives

$$\liminf_{h\to\infty} I(u_h, \Omega) \geqq J_\Gamma(u, \Omega) + \int_{\Omega_\delta \setminus \bar{\Omega}} W^{**}(\nabla u_0) - W(\nabla u_0) dx\,.$$

On the other hand, as $\delta \to 0$ we have

$$\int_{\Omega_\delta \setminus \Omega} W(\nabla u_0) dx \to 0\,,$$

since $\nabla u_0 \in W^{1,2}$ and $W(\beta) \leqq c|\beta|^2$. Finally, continuity of the normal component follows from the compactness result of Lemma 3.14. This concludes the proof of the lower bound.

We now turn to the upper bound. We follow the argument of ANZELLOTTI & GIAQUINTA [2]. The main idea is to first modify u so that it takes the full boundary condition, not only the normal component. This is done by moving the tangential discontinuity occurring on Γ slightly inside the domain. This is the point where the C^2-smoothness of the boundary $\partial\Omega$ is relevant. Let a be such that in the set

$$\Omega_a = \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) < a\}$$

the function $x \to \operatorname{dist}(x, \partial\Omega)$ is C^1, the projection $x \to Px$ on the boundary is well defined and C^1, and $\nabla \operatorname{dist}(x, \partial\Omega)(x) = \nu(Px)$. ANZELLOTTI & GIAQUINTA have shown (Theorem 1.8 of [2], see also Theorem 5.2 of [3]) that for any boundary

value $u-u_0$ with zero normal component, a function $\psi \in U(\Omega)$ can be found such that

$$\psi = \begin{cases} u-u_0 & \text{on } \Gamma\,, \\ 0 & \text{on } \partial\Omega \setminus \Gamma\,, \end{cases}$$

$$\operatorname{supp}\psi \subset \Omega_a \qquad \text{and} \qquad \psi(x)\cdot\nabla \operatorname{dist}(\cdot,\partial\Omega)(x) = 0 \text{ on } \Omega_a\,.$$

We now set

$$\eta_k(x) = \max\,(0,\, 1-k\,\operatorname{dist}(x,\partial\Omega)) \qquad \text{and} \qquad w_k = u+\eta_k\psi\,.$$

We have

$$Ew_k = Eu + \eta_k E\psi + \tfrac{1}{2}\,(\nabla\eta_k\otimes\psi + \psi\otimes\nabla\eta_k)$$

and in particular

$$\operatorname{div} w_k = \operatorname{div} u + \eta_k \operatorname{div}\psi\,,$$

since $\nabla\eta_k(x)$ is parallel to $\nabla\operatorname{dist}(x,\partial\Omega)$, which is orthogonal to $\psi(x)$.

We now claim that, as $k\to\infty$,

$$\int_\Omega W^{**}\left((\nabla\eta_k\otimes\psi)^{\mathrm{sym}}\right)dx \to \int_\Gamma W^\infty((u-u_0)\otimes\nu)d\mathcal{H}^2\,. \tag{3.17}$$

To see this, let ϕ be defined as $u-u_0$ on Γ (as usual, in the sense of traces) and zero on the rest of $\partial\Omega$. By the trace theorem there is a subset $E\subset(0,a)$ of full measure (i.e., $|E|=a$) such that

$$\int_{\partial\Omega} |\psi(x+b\nu(x)) - \phi(x)|\,d\mathcal{H}^2(x) \to 0 \qquad \text{as } b\to 0\,,\quad b\in E\,.$$

The first integral in (3.17) can be written as

$$\begin{aligned}&\int_\Omega W^{**}\left((\nabla\eta_k\otimes\psi)^{\mathrm{sym}}\right)dx \\ &\quad = \int_{\partial\Omega} d\mathcal{H}^2 \int_0^{1/k} W^{**}\left(k(\nu(Px)\otimes\psi(x+b\nu(x))^{\mathrm{sym}}\right)\,J\,db,\end{aligned}$$

where J is the suitable Jacobian determinant, which converges uniformly to unity for small k since the boundary is C^2. The argument of W^{**} is traceless, therefore W^{**} has linear growth, and by the L^1 convergence above we can replace $\psi(x+b\nu(x))$ with $\phi(x)$ in its argument, in the limit. This concludes the proof of (3.17).

At the same time,

$$\int_{\Omega_{1/k}} W^{**}\,(Eu+\eta_k E\psi)\;dx \to 0$$

since they are both summable. It follows that

$$J(w_k, \Omega) \to J_\Gamma(u, \Omega)$$

with w_k satisfying the full Dirichlet boundary conditions, i.e., $w_k = u_0$ on Γ. Then, the proof is concluded as the one of Theorem 3.3. In particular, we have shown there that each w_k can be approximated by a sequence $v_h^{(k)}$ such that

$$v_h^{(k)} \to w_k \text{ in } L^1\,, \qquad I(v_h^{(k)}, \Omega) \to I(w_k, \Omega)\,, \qquad v_h^{(k)} = w_k \text{ on } \partial\Omega\,.$$

If we take a diagonal subsequence the proof is concluded. □

4. Nonlocal problem

In this section we extend the analysis to a nonlocal problem which includes a singular perturbation representing the line energy of dislocations, as the functional (2.4). This permits us to incorporate a length scale into the problem and therefore to study size effects, as for example the Hall-Petch dependence on grain size in polycrystals. We consider a cubic grain of material $\Omega_L = (0, L)^3$ embedded in an elastic matrix, on which an average shear γ is imposed. For simplicity we focus on the case where only two slip systems are active, and consider only one scalar component of the deformation field. The assumption that the matrix can only deform elastically is appropriate for a polycrystal since neighboring grains with a different orientation cannot deform plastically along the considered direction. We seek a deformation $u : \Omega_L \to \mathbb{R}$ and a plastic strain $\beta^p : \Omega_L \to \mathbb{R}^3$ which minimize the free energy

$$E(u, \beta^p, \sigma, \mu, \tau, L, \gamma) = \int_{\Omega_L} |\nabla u - \beta^p|^2 dx + \tau \int_{\Omega_L} |\beta^p| dx + \sigma \int_{\Omega_L} |\nabla \times \beta^p| + \mu \, \|u - \gamma x_1\|^2_{H^{1/2}(\partial\Omega_L)} \quad (4.1)$$

subject to the side conditions $\beta_1^p = \pm\beta_2^p$ and $\beta_3^p = 0$ a.e.. We remark that, at variance with the previous section, here u is a scalar and β^p a vector. Here and below we use the shorthand notation

$$\int_\Omega |\nabla \times \beta^p| = \frac{1}{2} \int_\Omega |(\partial_1 + \partial_2)(\beta_1^p - \beta_2^p)| + |(\partial_1 - \partial_2)(\beta_1^p + \beta_2^p)| + |\partial_3(\beta_1^p + \beta_2^p)| + |\partial_3(\beta_1^p - \beta_2^p)| \quad (4.2)$$

where the norms on the right are intended in the sense of measures, i.e., for example

$$\int_\Omega |(\partial_1 - \partial_2)(\beta_1^p + \beta_2^p)| = \sup \int_\Omega (\phi_{,1} - \phi_{,2})(\beta_1^p + \beta_2^p) dx\,.$$

The supremum is here taken over all $\phi \in C_0^0(\Omega, [-1, 1])$, and the (distributional) partial derivatives are denoted by $\partial_1\phi = \phi_{,1} = \partial\phi/\partial x_1$. It is easy to check that for smooth functions β^p which satisfy the side condition $\beta_1^p = \pm\beta_2^p$, $\beta_3^p = 0$ this

coincides with the classical interpretation of $|\nabla \times \beta^p|$ as the norm of the curl of β^p. We remark, however, that (4.2) does not coincide with the norm of the distributional curl for generic functions of bounded variation which satisfy the side condition. Indeed, consider for example the field given by

$$\bar{\beta}^p = \begin{cases} (1,1,0)^T & \text{if } x_2 \geqq 0, \\ (1,-1,0)^T & \text{if } x_2 < 0\,. \end{cases}$$

The distributional curl of $\bar{\beta}^p$ vanishes, since $\bar{\beta}^p = \nabla(x_1 + |x_2|)$, but the norm defined in (4.2) does not. From the point of view of relaxation, it is easy to approximate $\bar{\beta}^p$ with smooth curl-free vector fields, e.g., by mollification, but this is impossible if the constraint is also considered. An approximation with smooth vector fields which satisfy the constraint and for which the quantity in (4.2) is continuous is instead easy. Namely, we first insert a small region where the vector field vanishes, as for example in

$$\beta^p_\varepsilon = \begin{cases} (1,1,0)^T & \text{if } x_2 > \varepsilon\,, \\ 0 & \text{if } -\varepsilon < x_2 < \varepsilon\,, \\ (1,-1,0)^T & \text{if } x_2 < -\varepsilon\,. \end{cases}$$

Then, we can mollify separately for positive and negative x_2, still keeping the zero boundary condition on the plane $x_2 = 0$, and finally take a diagonal subsequence. This shows that the definition (4.2) is appropriate for the curl of a distribution obtained by relaxation subject to the side condition $\beta^p_1 = \pm\beta^p_2$, $\beta^p_3 = 0$. Physically, this corresponds to assuming that a thin elastic layer is always present between regions deformed along the two different slip systems. In other words, dislocations generated by the two slip systems do not annihilate each other, even if they have opposite Burgers vector.

In (4.1) a global multiplicative factor representing the typical elastic constant of the material has been set to unity for simplicity. The material parameter σ represents the line energy of dislocations, or equivalently the surface energy of dislocation walls, called T/b in (2.4), and γ represents the average shear deformation imposed on the material. The parameter μ represents the relative strength of the matrix (i.e., of the rest of the material, located in $\mathbb{R}^3 \setminus \Omega_L$) with respect to the considered grain. The squared $H^{1/2}$ seminorm on the boundary used here is equivalent to the squared L^2 norm of the optimal continuation of ∇u on the complement of Ω_L. In the limit $\mu \to \infty$ we expect to recover the hard Dirichlet boundary conditions, namely, $u(x) = \gamma x_1$ on $\partial\Omega_L$.

By scaling we can eliminate the parameters L and γ. Precisely, we set

$$\tilde{u}(x) = \frac{1}{\gamma L} u(Lx)\,, \qquad \tilde{\beta}^p(x) = \frac{1}{\gamma}\beta^p(Lx)\,,$$

and obtain

$$E(u, \beta^p, \sigma, \mu, \tau, L, \gamma) = L^3\gamma^2 E\left(\tilde{u}, \tilde{\beta}^p, \frac{\sigma}{\gamma L}, \mu, \frac{\tau}{\gamma}, 1, 1\right).$$

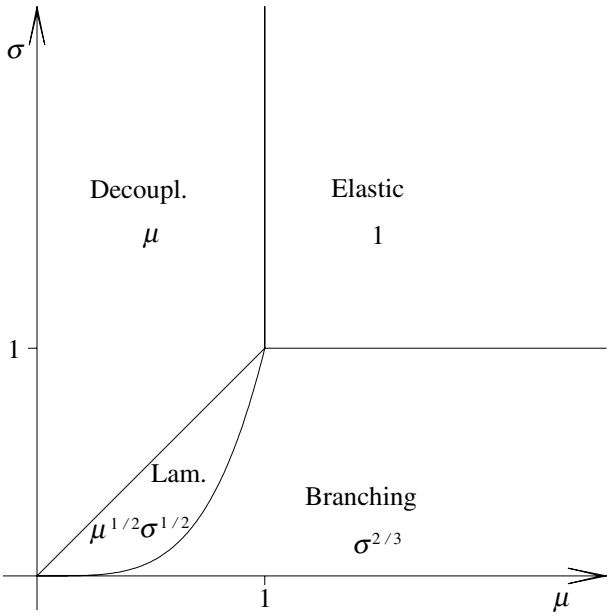


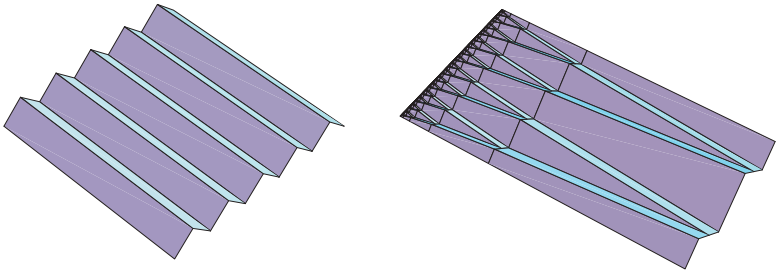
Fig. 4.1. Idealized phase diagram in the $(\mu, \tilde{\sigma})$ plane for $\tau = 0$, with all constants set to unity, as in (4.3).

We now define $\tilde{\sigma} = \sigma/\gamma L$, $\tilde{\tau} = \tau/\gamma$, and study the infimum of the reduced energy $\tilde{E}(u, \beta^p, \tilde{\sigma}, \mu, \tilde{\tau}) = E(u, \beta^p, \tilde{\sigma}, \mu, \tilde{\tau}, 1, 1)$ over u and β^p. Our main result is that its scaling behavior is the same as that of

$$E_0(\tilde{\sigma}, \mu, \tilde{\tau}) = \min\left(1, \mu, \tilde{\tau} + \mu^{1/2}\tilde{\sigma}^{1/2}, \tilde{\tau} + \tilde{\sigma}^{2/3}\right). \tag{4.3}$$

This shows that four regimes are present, which are discussed in Section 4.2 below and illustrated, for the simplest case $\tau = 0$, in Fig. 4.1. At large $\tilde{\sigma}$ (i.e., $\sigma/\gamma L$) no microstructure can form, and the crystal deforms uniformly. If μ is large, the coupling to the matrix is also strong, and this results in a purely elastic regime. If the coupling is weak, i.e., μ is small, the grain decouples from the rest of the crystal, and does not follow the average deformation. For small $\tilde{\sigma}$ (i.e., $\sigma/\gamma L$) the grain deforms plastically, and the macroscopic imposed deformation is realized by forming fine mixtures between regions deformed along the two slip systems. Depending on the value of the coupling constant μ, this can either be a laminar structure or a branched structure with finer mixtures closer to the boundary. These two patterns, which are illustrated in Fig. 4.2, have been used in a number of different problems where a nonconvex bulk energy density with multiple minima is accompanied by boundary conditions, or forcing terms, which favor some convex combination of the minima, by a differential condition favoring a certain orientation of the interfaces, and by a singular perturbation that penalizes very fine structures. Oscillations which refine towards the boundary as a possible competitor to uniform oscillations have been first used in the discussion of branched domains in the intermediate state

Dislocation Microstructures



(a) (b)

Fig. 4.2. Two different kinds of fine-scale structures may form. (a) An essentially one-dimensional pattern, known as laminate, minimizes the bulk energy but realizes boundary conditions only up to a small error. (b) A two-dimensional domain-branching pattern can accommodate Dirichlet boundary conditions, and still have coarse oscillations in the interior, at the expense of higher bulk energy in the transition layers.

of type-I superconductors by LANDAU back in 1938 [34, 35]. Mathematically, a transition between a laminar regime at weak coupling to the outside material and a branching pattern when the coupling is stronger was first proved in a simplified model of martensitic phase transitions by KOHN & MÜLLER in 1992 and 1994 [32, 33], and later refined in [13]. Since then, analogous results have been obtained for models of uniaxial ferromagnets [10, 11], of blistering in compressed thin films [29, 7, and references therein], and of flux domain structures in the intermediate state of type-I superconductor plates [12].

4.1. Energy scaling

Theorem 4.1. *There are constants c, c' such that, for all $\sigma > 0$, $\mu > 0$, $\tau \geqq 0$, $L > 0$, $\gamma > 0$,*

$$cE_0(\tilde{\sigma}, \mu, \tilde{\tau}) \leqq \frac{1}{L^3\gamma^2} \inf E(u, \beta^p, \sigma, \mu, \tau, L, \gamma) \leqq c' E_0(\tilde{\sigma}, \mu, \tilde{\tau})$$

where the infimum is taken over all u and β^p which obey the side condition $\beta_1^p = \pm\beta_2^p$, $\beta_3^p = 0$ a.e., $\tilde{\sigma} = \sigma/\gamma L$, $\tilde{\tau} = \tau/\gamma$, and

$$E_0(\tilde{\sigma}, \mu, \tilde{\tau}) = \min\left(1, \mu, \tilde{\tau} + \mu^{1/2}\tilde{\sigma}^{1/2}, \tilde{\tau} + \tilde{\sigma}^{2/3}\right).$$

Proof. By the scaling mentioned above, it is clearly sufficient to prove the result for $L = \gamma = 1$, and to work with the reduced energy $\tilde{E}$. We state the proof separately for the upper and lower bounds.

Upper bound. We shall prove that the energy is bounded from above by a constant times each of the four terms entering E_0, and hence also by their minimum. This requires four different constructions, two of which are trivial. We proceed in order of increasing complexity.

The first upper bound corresponds to the purely elastic deformation obtained by setting $\beta^p = 0$, $u(x) = x_1$. A direct substitution gives $\tilde{E}(x_1, 0, \sigma, \mu, \tau) = 1$.

The second upper bound corresponds to no deformation at all, i.e., to a decoupling of the grain from the matrix. Setting $\beta^p = u = 0$, we get $\tilde{E}(0, 0, \sigma, \mu, \tau) = c\mu$ for some $c > 0$.

The third construction is the laminate, as illustrated in Fig. 4.2(a). This is essentially the same construction used in the previous section for the local problem. The difference here is that the boundary conditions need to be satisfied only approximately, whereas the surface energy needs to be accounted for. Therefore we need to choose the optimal length scale for the oscillation. Precisely, given a positive integer n, we set $\beta^p(x) = \nabla u(x) = (1, 1, 0)$ if nx_2 has an odd integer part, and $\beta^p(x) = \nabla u(x) = (1, -1, 0)$ else. The first term in E vanishes, the second equals $\tau\sqrt{2}$ (since $|\beta^p| = \sqrt{2}$), and the third equals $2\sigma n$ (since there are n planar interfaces of unit area). To estimate the last term, we recall that by a standard interpolation inequality for any v we have

$$\|v\|^2_{H^{1/2}(\partial\Omega_L)} \leqq c\,\|v\|_{H^1(\partial\Omega_L)} \cdot \|v\|_{L^2(\partial\Omega_L)} \,.$$

Since $|u - x_1| \leqq 1/n$ and $|\nabla u| \leqq 2$, setting $v = u - x_1$ we see that the squared $H^{1/2}$ seminorm is controlled by c/n, and hence the boundary term is controlled by $c\mu/n$. Combining the four terms we get $E \leqq c(\tau + \sigma n + \mu/n)$, and choosing $n = \mu^{1/2}\sigma^{-1/2}$ we get the result. This construction only needs to be done in the regime $\sigma < \mu$, hence $n > 1$, and rounding to an integer only affects the estimate by a factor. We remark that the period of the laminar pattern is given by

$$l = \frac{1}{n} = \left(\frac{\sigma}{\mu}\right)^{1/2} .$$

Finally, the fourth upper bound is obtained with a branched construction, as illustrated in Fig. 4.2(b). This is a more complex construction, and for greater clarity we present it first in two dimensions (i.e., on a section at constant x_3 in the central part of the sample) and then extend it to three dimensions. This construction is characterized by the fact that it can accommodate a large oscillation period in the bulk of the sample while reaching the exact boundary conditions, i.e., with $u = \gamma x_1$ on $\partial\Omega_L$. Therefore the resulting energy bound does not depend on μ.

The basic building block is the transition from a single oscillation to a double oscillation (period-doubling step), as represented in Fig. 4.3(a). Consider for definiteness a rectangle of width k and height $2h$, with the origin in the midpoint of the left side. The central triangle in Fig. 4.3(b) has (vertical) basis h and (horizontal) height k. The plastic deformation takes only the two values $(1, \pm 1)$, and the elastic field u takes the values given in Fig. 4.3(a) (the third component of β^p, which vanishes by the side condition, is here dropped from the notation). We now evaluate the energy inside this $k \times 2h$ rectangle. The elastic energy is the integral of $|\nabla u - \beta^p|^2$. The latter equals $(h/k)^2$ per unit area inside the central triangle, and zero outside, hence the total elastic energy is $h^3/2k$. The two horizontal interfaces

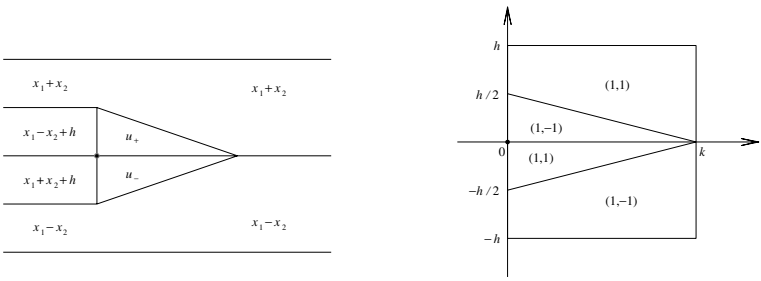


Fig. 4.3. Branching construction. (a) Sketch of the transition between a double laminate and a single one. The value of u is given in each piece where it is affine, and $u_- = x_1 + x_2 + h(1 - x_1/k)$, $u_+ = x_1 - x_2 + h(1 - x_1/k)$. The dot marks the origin of the chosen axis. (b) The basic block of size $(0, k) \times (-h, h)$ used for the branching construction. The values give β^p in the four regions.

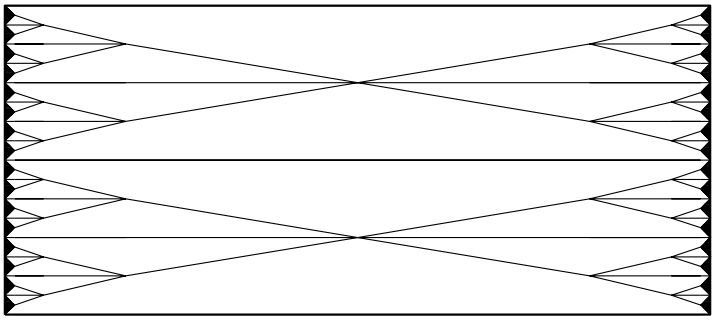


Fig. 4.4. Branching construction, global picture. Three steps of refinement are shown. The black triangles are the boundary layer where no branching takes place. In the text only the left half of the construction is discussed explicitly, the rest is symmetric.

have total energy $2 \cdot 2k\sigma$. Each of the oblique interfaces has energy controlled by $2\sigma(k + h)$. The total energy in the rectangle is then controlled by

$$\frac{h^3}{2k} + \sigma\,(4k + 4(k + h)) + hk\tau\sqrt{2}\,. \tag{4.4}$$

Optimization with respect to the horizontal width k gives $k = h(h/\sigma)^{1/2}/4$, and (assuming $h \geqq \sigma$) an energy bound on each rectangle of

$$E_{\text{rect,2D}} \leqq ch^{3/2}\sigma^{1/2} + 4hk\tau\,.$$

In a second step, the various rectangles are combined together to achieve the branching pattern represented in Fig. 4.4. At the i-th iteration step the period is given by

$h_i = h_0 2^i$, and there are $1/h_i$ rectangles like the one in Fig. 4.3(b). The total energy for the i-th iteration is controlled by

$$E_{2\mathrm{D}}^{(i)} \leqq c h_i^{1/2} \sigma^{1/2} + 4k\tau \,.$$

At the left and right boundaries there is a series of triangles where $\beta^p = 0$ and u interpolates between the oscillatory value in the interior and the affine boundary data. These triangles have basis h_0 given by the smallest period reached by the branching construction, and height also of order h_0. This first layer has surface energy controlled by σ, and elastic energy controlled by its area, which is of order h_0. Therefore its total energy is

$$E_{2\mathrm{D}}^{(0)} \leqq c(h_0 + \sigma + \tau) \,.$$

Summing over all periods, we can estimate the energy of the two-dimensional branched construction by

$$E_{\mathrm{br}} = E_{2\mathrm{D}}^{(0)} + \sum_{i=1}^{N} E_{2\mathrm{D}}^{(i)} \leqq c \left[h_0 + \sigma + \tau + (h_0 \sigma)^{1/2} 2^{N/2} \right] .$$

The value of N is determined by the length of the sample in the x_1 direction,

$$1 = \sum_{i=1}^{N} k_i = \sum_{i=1}^{N} c \frac{h_0^{3/2}}{\sigma^{1/2}} 2^{3i/2} = c \frac{h_0^{3/2}}{\sigma^{1/2}} 2^{3N/2} \,.$$

The total energy satisfies

$$E_{\mathrm{br}} \leqq c h_0 + c\sigma + c\sigma^{2/3} + c\tau \,.$$

We finally have to choose h_0, which needs to fulfill $h_0 \geqq \sigma$ (this was used after equation (4.4)). The optimal value is clearly $h_0 = \sigma$, and gives for the optimal branching construction the scaling estimates

$$h_i = \sigma 2^i \qquad k_i = \sigma 2^{3i/2} \qquad E_{\mathrm{br}} \leqq c\sigma^{2/3} + c\tau \,.$$

This construction is admissible only for small σ, i.e., in the regime $h_0 \leqq 1$, $N \geqq 1$. In the center of the sample the oscillation period scales as $\sigma^{1/3}$.

Now we generalize to three dimensions. The idea is that for intermediate values of x_3 the above construction applies with no changes, and that for x_3 approaching the upper and lower boundaries the oscillations refine much as for x_1 approaching the left and right boundaries. For simplicity, we consider explicitly only the situation around the origin, i.e., present a construction on $(0, \infty)^3$; the other seven corners of the cube are treated analogously. Note that no refinement is needed approaching the face $x_2 = 0$, since this is parallel to the oscillation direction.

Let l_i be the value of x_1 where the i-th branching step takes place in the two-dimensional construction, $l_i = \sum_{j<i} k_j$. We define the regions

$$T_i = \left\{ x : l_i \leqq \min(x_1, x_3) \leqq l_{i+1} \right\}$$

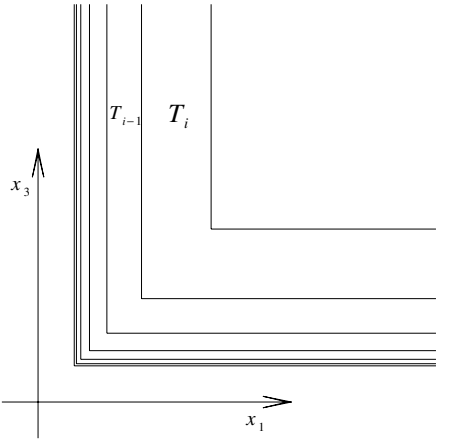


Fig. 4.5. Domains T_i in the (x_1, x_3) plane in which the three-dimensional branching takes place.

where branching between period h_i and period $h_{i+1} = 2h_i$ takes place (see Fig. 4.5). Precisely, on the surface $\min(x_1, x_3) = l_i$ the field β^p oscillates in x_2 on a scale h_i between the values $(1, \pm 1, 0)$; analogously u oscillates between $x_1 + x_2 + c$ and $x_1 - x_2 + c$ on the same scale, with constants chosen to guarantee continuity. The same holds for all i.

We now show how to construct the branching step in region T_i. If $x_3 \geqq x_1$, the above construction applies with no changes, and no dependence on x_3 is present. If instead $x_1 \geqq x_3$, a very similar construction applies. Precisely, the domain is subdivided in an x_1-independent way as in Fig. 4.3(b), where now the horizontal axis represents x_3 (and the vertical one still x_2). The values of β^p in the different triangles remain the same (with vanishing third component); the same expression holds for u on the boundary and in the two outer regions. Then, u is defined in the two triangles by linear interpolation between the values at the corners. Precisely, we find that the expressions for u_- and u_+ in Fig. 4.3(a) are replaced by $\tilde{u}_- = x_1 + x_2 + h(1 - x_3/k)$, $\tilde{u}_+ = x_1 - x_2 + h(1 - x_3/k)$. The remaining expressions for u are unchanged. Note that this construction gives a continuous u on the line $x_1 = x_3$. The energy is the same as in the two-dimensional case, after multiplication by the length in the third direction (which is unity), and inclusion of an additional interface in β^p on the surface $x_1 = x_3$, which gives a negligible energy contribution of order $h_i\sigma$.

Combining the different pieces, and inserting boundary layers as above, we get a function u which obeys $u(x) = x_1$ on $\partial(0, 1)^3$ and has energy controlled by

$$E_{\mathrm{br}} \leqq c\sigma^{2/3} + c\tau \,.$$

This concludes the proof of the upper bound.

Lower bound. The proof of the lower bound is based on a subdivision of the domain in small parallelepipeds, and on the rigidity results of Lemmas 4.2 and 4.3 (below) applied to their sections. We start from the case $\tau = 0$.

For any $l < 1/2$, inside the square $(0,1)^2$ we can choose at least $l^{-2}/2$ squares with sides of length l and parallel to the lines $x_1 = x_2$ and $x_1 = -x_2$, respectively. Denote them by Q_l^i. Let E_i be the amount of energy contained in the set $Q_l^i \times \mathbb{R}$, defined by

$$E_i = \|\nabla u - \beta^p\|^2_{L^2(Q_l^i \times (0,1))} + \sigma \|\nabla \times \beta^p\|_{L^1(Q_l^i \times (0,1))} + \mu \|u - x_1\|^2_{H^{1/2}(Q_l^i \times \{0,1\})}$$

(the L^1 norm is understood in the sense of (4.2). Due to the superadditivity of the squared $H^{1/2}$ seminorm, which can be easily checked using the double-integral representation, we get

$$E \geqq \sum_i E_i \geqq \frac{1}{l^2} \min_i E_i \,.$$

Further, the side condition $\beta_1^p = \pm \beta_2^p$, $\beta_3^p = 0$ is satisfied a.e. in each parallelepiped.

We now choose an optimal section of an optimal parallelepiped, i.e., choose i and x_3 so that $E_i = \min_j E_j$ and

$$\|\nabla u - \beta^p\|^2_{L^2(Q_l^i \times \{x_3\})} + \sigma \|\nabla \times \beta^p\|_{L^1(Q_l^i \times \{x_3\})} \leqq E_i \,,$$

with the side condition satisfied a.e. in $Q_l^i \times \{x_3\}$.

By Lemma 4.3 there is a function f of the form $g(x_1 + x_2)$ or $g(x_1 - x_2)$ such that

$$\|u - f\|_{L^1(Q_i \times \{x_3\})} \leqq c l^2 E_i^{1/2} + c \frac{l^2 E_i}{\sigma} \,.$$

Combining the Poincaré inequality and the L^2-L^1 embedding we get

$$\begin{aligned} \|u - f\|_{L^1(Q_i \times \{0\})} &\leqq \|u - f\|_{L^1(Q_i \times \{x_3\})} + \|\partial_3 u\|_{L^1(Q_i \times (0,1))} \\ &\leqq \|u - f\|_{L^1(Q_i \times \{x_3\})} + l \|\partial_3 u\|_{L^2(Q_i \times (0,1))} \\ &\leqq c l E_i^{1/2} + c \frac{l^2 E_i}{\sigma} \,, \end{aligned}$$

since $|\partial_3 u|^2 \leqq |\nabla u - \beta^p|^2$ and $l \leqq 1$.

Finally, we use Lemma 4.2 on $Q_i \times \{0\}$. We get

$$\|u - f\|_{L^1(Q_i \times \{0\})} + \|u - x_1\|^2_{H^{1/2}(Q_i \times \{0\})} \geqq c l^3 \,.$$

Combined with the previous inequality and the definition of E_i, this gives

$$2 l E_i^{1/2} + \frac{l^2 E_i}{\sigma} + \frac{E_i}{\mu} \geqq c l^3 \,,$$

i.e.,

$$E \geqq \frac{E_i}{l^2} \geqq c \min\left(l^2, \frac{\sigma}{l}, l\mu\right)$$

for any $l < 1/2$. It only remains to choose the appropriate values of l in the four regimes. If $\sigma \geqq \min(1, \mu)$ we choose $l = 1/2$, and get $E \geqq c \min(1, \mu)$. This covers the two "simple" regimes. In the lamination regime $\mu^3 \leqq \sigma \leqq \mu \leqq 1$, we choose $l = \sigma^{1/2}\mu^{-1/2}$, and get $E \geqq \sigma^{1/2}\mu^{1/2}$. In the branching regime $\sigma \leqq \min(1, \mu^3)$, we choose $l = \sigma^{1/3}$ and get $E \geqq \sigma^{2/3}$. This concludes the proof if $\tau = 0$.

Now we prove the result for large τ, then the thesis will follow by interpolation. As above, we choose a "good" section x_3, such that the restriction of the energy to $(0, 1)^2 \times \{x_3\}$ is as low as on average. Combining the first two terms of the energy we obtain

$$\begin{aligned}\|\nabla u\|_{L^1((0,1)^2\times\{x_3\})} &\leqq \|\nabla u - \beta^p\|_{L^2((0,1)^2\times\{x_3\})} + \|\beta^p\|_{L^1((0,1)^2\times\{x_3\})} \\ &\leqq E^{1/2} + \frac{E}{\tau}\,.\end{aligned}$$

By the Poincaré inequality there is a constant $c \in \mathbb{R}$ such that

$$\|u - c\|_{L^1((0,1)^2\times\{x_3\})} \leqq E^{1/2} + \frac{E}{\tau}\,.$$

Now, as above, we use the $\partial_3 u$ part of the first term in the energy on $(0, 1)^2 \times (0, x_3)$ to get

$$\|u - c\|_{L^1((0,1)^2\times\{0\})} \leqq 2E^{1/2} + \frac{E}{\tau}\,,$$

and from Lemma 4.2 with $f = c$ and $l = 1$ we get

$$2E^{1/2} + \frac{E}{\tau} + \frac{E}{\mu} \geqq c\,.$$

Equivalently,

$$E \geqq c \min(1, \mu, \tau)\,,$$

which is the desired bound for large τ. Finally, the thesis follows by averaging between the two bounds (i.e., from $E \geqq \min(x, y)$ and $E \geqq \min(x, y')$ we get $E \geqq \min(x, (y + y')/2)$). □

Finally we present the two interpolation lemmas used in the proof.

Lemma 4.2. *There is a constant $c > 0$ such that for any $u : Q_l \to \mathbb{R}$, $f : \mathbb{R} \to \mathbb{R}$, where Q_l is a square of side l, the following inequality holds:*

$$\|u(x_1, x_2) - f(x_1 + x_2)\|_{L^1(Q_l)} + \|u(x_1, x_2) - x_1\|^2_{H^{1/2}(Q_l)} \geqq cl^3\,.$$

The same holds if $f(x_1 + x_2)$ is replaced by $f(x_1 - x_2)$.

Proof. By scaling $\tilde{u}(x) = lu(x/l)$, and $\tilde{f}(x) = lf(x/l)$, it is clearly sufficient to prove the statement for $l = 1$. We proceed by contradiction. If the thesis were false, there would be sequences u_j and f_j such that $u_j - f_j \to 0$ in $L^1(Q_1)$, and $u_j \to x_1$ in $H^{1/2}(Q_1)$ and hence $u_j - c_j \to x_1$ in $L^1(Q_1)$, for some constants c_j. But then, $f_j(x_1 + x_2) - c_j \to x_1$ in $L^1(Q_1)$, a contradiction. □

Lemma 4.3. *Let $Q_l = \{|x_1 \pm x_2| \leqq l/\sqrt{2}\}$ be a square of side l, and consider functions $u : Q_l \to \mathbb{R}$ and $\beta^p : Q_l \to \mathbb{R}^2$, with $\beta^p_1 = \pm\beta^p_2$ a.e.. Then, there is $f : (-l/\sqrt{2}, l/\sqrt{2}) \to \mathbb{R}^2$ such that*

$$\min\left(\|u(x_1,x_2) - f(x_1+x_2)\|_{L^1(Q_l)}, \|u(x_1,x_2) - f(x_1-x_2)\|_{L^1(Q_l)}\right) \leqq l^2\|\nabla u - \beta^p\|_{L^2(Q_l)} + l^2\|\nabla \times \beta^p\|_{L^1(Q_l)}\,.$$

The last term is understood in the sense of (4.2).

Proof. By the same scaling as above, it is sufficient to prove the thesis for $l = 1$. Let (ξ, η) be coordinates rotated by 45 degrees with respect to (x_1, x_2), such that the domain Q_1 becomes $Q = \{0 \leqq \xi, \eta \leqq 1\}$. In these coordinates, the side condition requires that at a.e. point either $\beta^p_\xi = (\beta^p_1 + \beta^p_2)/\sqrt{2}$ or $\beta^p_\eta = (\beta^p_1 - \beta^p_2)/\sqrt{2}$ vanishes. We define

$$\omega^{(\xi)} = \left\{\xi \in (0,1) \text{ such that } \beta^p_\xi(\xi,\eta) \neq 0 \text{ for a.e. } \eta \in (0,1)\right\},$$
$$\omega^{(\eta)} = \left\{\eta \in (0,1) \text{ such that } \beta^p_\eta(\xi,\eta) \neq 0 \text{ for a.e. } \xi \in (0,1)\right\},$$

and $\omega = \omega^{(\xi)} \times \omega^{(\eta)} \subset (0,1)^2$. These definitions ensure that $\beta^p_\xi \neq 0$ almost everywhere on ω, and the same for β^p_η. Since by the side condition for almost every point of Q at least one of β^p_ξ and β^p_η vanishes, the set ω is a null set (with respect to the two-dimensional Lebesgue measure), and hence at least one of the two sets $\omega^{(\xi)}$ and $\omega^{(\eta)}$ has vanishing one-dimensional measure. Assume for concreteness that $\omega^{(\xi)}$ is a null set. Then, for a.e. $\xi \in (0,1)$ there is a set $\theta(\xi) \subset (0,1)$ of positive measure such that $\beta^p_\xi = 0$ on $\{\xi\} \times \theta(\xi)$. It follows that, for a.e. $\eta \in (0,1)$,

$$|\beta^p_\xi(\xi,\eta)| \leqq \int_0^1 d\eta' |\partial_\eta \beta^p_\xi|$$

and hence, integrating first with respect to η and then with respect to ξ,

$$\int_Q |\beta^p_\xi(\xi,\eta)| \leqq \int_Q |\partial_\eta \beta^p_\xi|\,.$$

In these coordinates the definition (4.2) reads $|\nabla \times \beta^p| = |\partial_\eta \beta^p_\xi| + |\partial_\xi \beta^p_\eta|$. Therefore

$$\int_Q |\partial_\xi u| \leqq \int_Q |\partial_\xi u - \beta^p_\xi| + \int_Q |\beta^p_\xi| \leqq \|\nabla u - \beta^p\|_{L^2(Q)} + \int_Q |\nabla \times \beta^p|.$$

Let $f(\eta) = u(0,\eta)$. Then

$$\int_Q |u(\xi,\eta) - f(\eta)| \leqq \int_Q |\partial_\xi u|$$

and the proof is concluded. In the other case, i.e., if $\omega^{(\eta)}$ is a null set, we get the same with $f(\xi) = u(\xi, 0)$. □

4.2. Discussion of the phase diagram

The estimate of the energy (4.3) shows that the yield strength τ only enters through special combinations, namely,

$$\tilde{\tau} + \mu^{1/2}\tilde{\sigma}^{1/2} \qquad \text{and} \qquad \tilde{\tau} + \tilde{\sigma}^{2/3}\,.$$

Both expressions have a very simple interpretation. Indeed, let l be the length scale of the microstructure, $l = \tilde{\sigma}/\mu^{1/2}$ in the first case and $l = \tilde{\sigma}^{1/3}$ in the second one (see constructions above). Then, both expressions can be written in the common form

$$\tilde{\tau} + \frac{\tilde{\sigma}}{l}\,.$$

The same relation holds in unscaled variables, if the appropriate expression for the unscaled l is used. This corresponds exactly to the scaling argument proposed by AUBRY & ORTIZ [4, equation (5.4)], based on which the dislocation line energy σ increases the effective yield strength of a material τ by an amount σ/l. In the following we shall focus on the geometric effects and for simplicity assume $\tau = 0$.

The phase diagram depicted in Fig. 4.1 is degenerate, in that all four phases meet at a point. This is merely a consequence of the fact that all constants have been set to unity. A more realistic model can be obtained by evaluating the upper bounds with appropriate constants. Whereas this procedure is not rigorous, and only provides upper bounds on the constants, it constitutes at a heuristic level a natural way to lift the degeneracy. Simple calculations show that, of the four constants, the one in the branching regime is the largest. Assume, for definiteness, that it is 50% larger than the others. Then we would estimate the energy with

$$E_1(\sigma, \mu, 0) = \min\left(1, \mu, \mu^{1/2}\sigma^{1/2}, \frac{3}{2}\sigma^{2/3}\right)\,. \tag{4.5}$$

Note that the statement of Theorem 4.1 holds also if E_0 is replaced with E_1 there, since they have the same scaling behavior. The phase diagram resulting from E_1 is illustrated in Fig. 4.6 (with the assumed factor $3/2$, if the ratio is bigger, the laminate construction gains additional weight at the expense of the branching one).

Consider now a typical monotonic loading experiment. The material parameters σ, μ, and L are fixed, whereas the strain γ is increased monotonically starting from zero. This means that $\tilde{\sigma} = \sigma/\gamma L$ decreases, starting from infinity, hence that we move down vertically in the phase diagram of Fig. 4.6, as indicated by the arrow. A different behavior is expected depending on the precise value of μ. To decide which is appropriate for a realistic experimental situation, the following two observations are helpful: (i) μ represents the relative strength of the other grains, hence is expected to be of order unity; (ii) for very small γ (i.e., very large $\tilde{\sigma}$) a uniform elastic deformation is expected, and therefore the appropriate phase is the elastic one, not the decoupled one. Hence the first phase transition encountered is the one

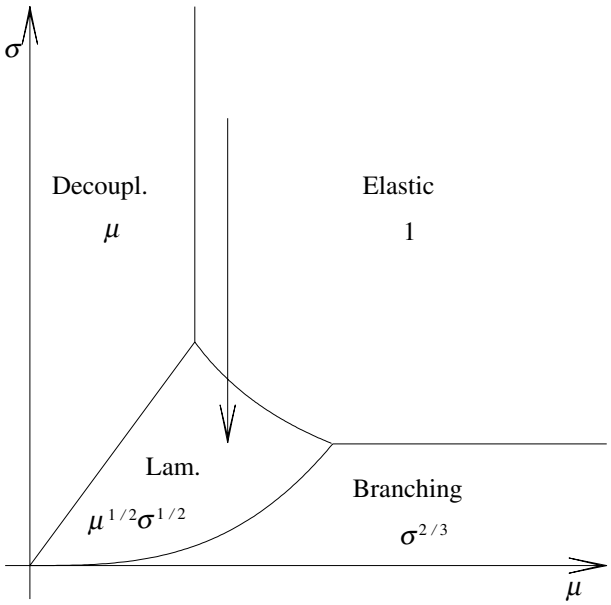


Fig. 4.6. Phase diagram in the $(\mu, \tilde{\sigma})$ plane, according to (4.5). The arrow denotes the direction of increasing deformation γ.

between elastic and laminate, which occurs at $\tilde{\sigma}\mu = 1$. After that, the energy per unit volume is given by

$$\frac{E_{\text{lam}}}{L^3} \sim \gamma^2(\mu\tilde{\sigma})^{1/2} = \frac{\gamma^{3/2}\mu^{1/2}\sigma^{1/2}}{L^{1/2}},$$

hence the strain, obtained by taking the derivative of the energy per unit volume with respect to γ, scales in the lamination regime as $(\gamma\mu\sigma/L)^{1/2}$. If the strain γ is increased further, we expect that the branching regime will eventually be reached, where the strain scales as $\gamma^{1/3}(\sigma/L)^{2/3}$.

From the point of view of the modeling of a polycrystalline material, the dependence of the stress on L corresponds to the dependence of the macroscopic stress on grain size. Therefore our model predicts that in polycrystals the stress beyond the elastic-to-plastic transition scales as the inverse square root of the grain size. This fact corresponds exactly to the experimentally known Hall-Petch law [20, 44].

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